

# Turán problems for digraphs avoiding distinct walks of a given length with the same endpoints

Zejun Huang,<sup>\*</sup> Zenhua Lyu,<sup>†</sup> Pu Qiao<sup>‡</sup>

## Abstract

Let  $n \geq 5$  and  $k \geq 4$  be positive integers. We determine the maximum size of digraphs of order  $n$  that avoid distinct walks of length  $k$  with the same endpoints. We also characterize the extremal digraphs attaining this maximum number when  $k \geq 5$ .

**Key words:** digraph, Turán problem, transitive tournament, walk

**AMS subject classifications:** 05C35, 05C20

## 1 Introduction

Turán problems concern the study of the maximum number, called Turán number, of edges in graphs containing no given subgraphs and the extremal graphs realizing that maximum. Mantel's theorem determines the maximum number of edges of triangle-free simple graphs as well as the unique graph attaining that maximum. Paul Turán [12, 13] generalized Mantel's theorem by determining the maximum number of edges of  $K_r$ -free graphs on  $n$  vertices and the unique graph attaining that maximum, where  $K_r$  denotes the complete graph on  $r$  vertices. Turán's theorem initiated the development of a major branch of graph theory, known as extremal graph theory [1, 10]. Most of the previous results in extremal graph theory concern undirected graphs and only a few extremal problems on digraphs have been investigated; see [1, 3, 4, 5, 6, 9]. In this paper we study extremal problems on digraphs.

We consider strict digraphs, i.e., digraphs without loops and parallel arcs. For digraphs, we abbreviate directed walks and directed cycles as walks and cycles, respectively. The

---

<sup>\*</sup>Institute of Mathematics, Hunan University, Changsha 410082, P.R. China. (mathzejun@gmail.com)

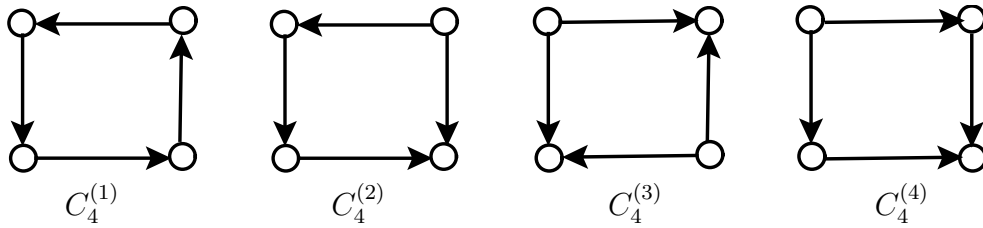
<sup>†</sup>College of Mathematics and Econometrics, Hunan University, Changsha 410082, P.R. China. (lyuzhh@outlook.com)

<sup>‡</sup>Department of Mathematics, East China Normal University, Shanghai 200241, China. (235711gm@sina.com)

number of vertices in a digraph is called its *order* and the number of arcs its *size*. We use  $\vec{K}_r$  and  $\vec{C}_r$  to denote the complete digraph and the directed cycle on  $r$  vertices.

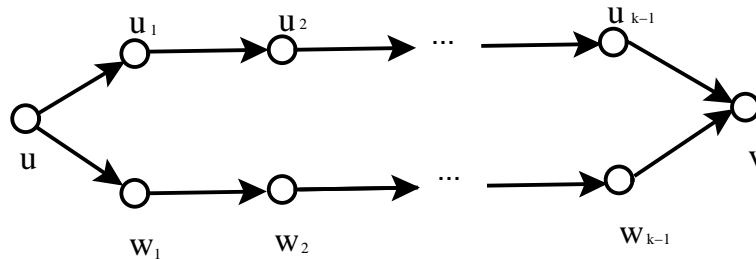
One natural Turán problem on digraphs is determining the maximum size of a  $\vec{K}_r$ -free strict digraph of a given order, which has been solved in [9].

Note that the  $k$ -cycle is a generalization of the triangle when we view a triangle as a 3-cycle in undirected graphs. Another generalization of Mantel's Theorem is the Turán problem for  $k$ -cycle-free graphs. However, this problem is difficult even for  $C_4$ -free graphs [7, 11]. An alternative direction on this problem is considering the orientations of  $C_k$ -free graphs. For example,  $C_4$  has the following orientations.



It is clear that a graph is  $C_4$ -free if and only if any of its orientation contains no copy of the above four digraphs. Hence the Turán number for  $C_4$ -free graphs is equal to that for  $\{C_2, C_4^{(1)}, C_4^{(2)}, C_4^{(3)}, C_4^{(4)}\}$ -free digraphs. For  $t \in \{1, 2, 3, 4\}$ , the Turán problem for  $C_4^{(t)}$ -free digraphs has independent interests; see [5]. We will consider a generalization of the Turán problem for  $C_4^{(4)}$ -free digraphs.

Given a positive integer  $k$ , we denote by  $\mathcal{F}_k$  the family of digraphs consisting of two different walks of length  $k$  with the same initial vertex and the same terminal vertex, which have the following diagram



where the vertices  $u, v, u_1, u_2, \dots, u_{k-1}, w_1, w_2, \dots, w_{k-1}$  can be duplicate but

$$(u_1, u_2, \dots, u_{k-1}) \neq (w_1, w_2, \dots, w_{k-1}).$$

We say a digraph  $D$  is  $\mathcal{F}_k$ -free if  $D$  contains no subgraph from  $\mathcal{F}_k$ . For any digraph  $D$  on the vertices  $1, 2, \dots, n$ ,  $D$  is  $\mathcal{F}_k$ -free if and only if there is at most one walk of length  $k$  from  $i$  to  $j$  for every pair of vertices  $i, j$ . Let  $ex(n, \mathcal{F}_k)$  be the maximum size of  $\mathcal{F}_k$ -free

strict digraphs of order  $n$  and  $Ex(n, \mathcal{F}_k)$  be the set of  $\mathcal{F}_k$ -free strict digraphs of order  $n$  with size  $ex(n, \mathcal{F}_k)$ . We study the following problem on strict digraphs.

**Problem 1.** *Given positive integers  $n$  and  $k$ , determine  $ex(n, \mathcal{F}_k)$  and  $Ex(n, \mathcal{F}_k)$ .*

When  $k = 1$ , it is clear that  $ex(n, \mathcal{F}_1) = n(n - 1)$  and the unique extremal digraph attaining  $ex(n, \mathcal{F}_1)$  is the complete digraph of order  $n$ . When  $k = 2$ ,  $\mathcal{F}_2$  consists of a unique digraph  $C_4^{(4)}$ .

In this paper, we always assume the order  $n \geq 5$ . We will determine  $ex(n, \mathcal{F}_k)$  for  $k \geq 4$  and characterize  $Ex(n, \mathcal{F}_k)$  for  $k \geq 5$ . The paper is organized as follows. Section 2 presents our main result Theorem 2, which determines  $ex(n, \mathcal{F}_k)$  for  $n \geq k + 4 \geq 8$  and characterizes  $Ex(n, \mathcal{F}_k)$  for  $n \geq k + 5 \geq 10$ ; section 3 presents the characterization of  $Ex(n, \mathcal{F}_k)$  for  $k \geq 4$  and  $n = k + 2, k + 3, k + 4$ ; section 4 presents the proof of Theorem 2; section 5 gives a discussion of the unsolved cases.

## 2 Main result

In order to present our main result, we need the follow notations and definitions. Let  $A$  be an  $n \times n$  matrix and  $\alpha = \{i_1, i_2, \dots, i_k\} \subseteq \{1, 2, \dots, n\}$ . We denote by  $A[\alpha]$  or  $A[i_1, i_2, \dots, i_k]$  the principal submatrix of  $A$  lying on its  $i_1$ -th,  $i_2$ -th,  $\dots$ ,  $i_k$ -th rows and columns, and denote by  $A(\alpha)$  or  $A(i_1, i_2, \dots, i_k)$  the principal submatrix of  $A$  obtained by deleting its  $i_1$ -th,  $i_2$ -th,  $\dots$ ,  $i_k$ -th rows and columns.

Let  $D = (\mathcal{V}, \mathcal{A})$  be a digraph with vertex set  $\mathcal{V} = \{v_1, v_2, \dots, v_n\}$  and arc set  $\mathcal{A}$ . Its *adjacency matrix*  $A_D = (a_{ij})$  is defined by

$$a_{ij} = \begin{cases} 1, & (v_i, v_j) \in \mathcal{A}; \\ 0, & \text{otherwise.} \end{cases} \quad (2.1)$$

Conversely, given an  $n \times n$  0-1 matrix  $A = (a_{ij})$ , we can define its digraph  $D(A) = (\mathcal{V}, \mathcal{A})$  on vertices  $v_1, v_2, \dots, v_n$  by (2.1), whose adjacency matrix is  $A$ .

Let  $A = (a_{ij})$  and  $B = (b_{ij})$  be matrices of order  $m$  and  $n$ , respectively.  $A \otimes B = (a_{ij}B)$  is the tensor product of  $A$  and  $B$ , whose order is  $mn$ . Denote by  $J_{m,n}$  and  $J_n$  the  $m \times n$  and  $n \times n$  matrices with all entries equal to one,

$$T_n = \begin{bmatrix} 0 & 1 & \cdots & 1 \\ & \ddots & \ddots & \vdots \\ & & 0 & 1 \\ & & & 0 \end{bmatrix}$$

the upper triangular tournament matrix of order  $n$ , and

$$\Pi_{m,n} = J_m \otimes T_n = \begin{bmatrix} T_n & \cdots & T_n \\ \vdots & \ddots & \vdots \\ T_n & \cdots & T_n \end{bmatrix}.$$

Two matrices  $A$  and  $B$  are said to be permutation similar if there is a permutation matrix  $P$  such that  $B = PAP^T$ , where  $P^T$  denotes the transpose of  $P$ . For two digraphs  $D_1$  and  $D_2$ ,  $A_{D_1}$  and  $A_{D_2}$  are permutation similar if and only if  $D_1$  and  $D_2$  are isomorphic.

A digraph of order  $n$  is called a *transitive tournament* if its adjacency matrix is permutation similar to  $T_n$ . Suppose  $m$  and  $t < n$  are nonnegative integers. We say a digraph of order  $mn + t$  is an  $(m, n, t)$ -completely transitive tournament if its adjacency matrix is permutation similar to  $\Pi_{m+1,n}(\alpha)$ , where  $\Pi_{m+1,n}(\alpha)$  is an  $(mn + t) \times (mn + t)$  principal submatrix of  $\Pi_{m+1,n}$  with  $\alpha \subseteq \{mn + 1, mn + 2, \dots, mn + n\}$  and  $|\alpha| = n - t$ . When  $t = 0$ , we see that a digraph of order  $mn$  is an  $(m, n, t)$ -completely transitive tournament if and only if its adjacency matrix is permutation similar to  $\Pi_{m,n}$ . Moreover, an  $(m, n, t)$ -completely transitive tournament is a subgraph of the  $(m + 1, n, 0)$ -completely transitive tournament.

Now we are ready to state our main result.

**Theorem 2.** *Let  $n = sk + t$  with  $s, k, t$  being nonnegative integers such that  $t < k$ . If  $n \geq k + 4 \geq 8$ , then*

$$ex(n, \mathcal{F}_k) = \binom{n}{2} - \binom{s}{2}k - st. \quad (2.2)$$

*Moreover, if  $n \geq k + 5 \geq 10$ , then a digraph  $D$  is in  $Ex(n, \mathcal{F}_k)$  if and only if  $D$  is an  $(s, k, t)$ -completely transitive tournament.*

We will also determine  $Ex(n, \mathcal{F}_k)$  for  $k \geq 4$  and  $n = k + 2, k + 3, k + 4$ , while  $ex(n, \mathcal{F}_k)$  for  $n \leq k + 3$  and  $Ex(n, \mathcal{F}_k)$  for  $n \leq k + 1$  can be easily deduced from [8].

From now on we deal with digraphs with no parallel arcs but allowing loops, and we use the same notations  $\mathcal{F}_k$ ,  $ex(n, \mathcal{F}_k)$  and  $Ex(n, \mathcal{F}_k)$  for digraphs allowing loops as for strict digraphs. We will give solutions to Problem 1 for digraphs allowing loops. The same results for strict digraphs follow straightforward, since there is no loop in these extremal digraphs from  $Ex(n, \mathcal{F}_k)$ .

### 3 $ex(n, \mathcal{F}_k)$ and $Ex(n, \mathcal{F}_k)$ for $n \leq k + 4$

For given integers  $n$  and  $k$ , denote by  $M_n\{0, 1\}$  the set of  $n \times n$  0-1 matrices,  $f(A)$  the number of ones in a 0-1 matrix  $A$ ,

$$\Gamma(n, k) = \{A \in M_n\{0, 1\} : A^k \in M_n\{0, 1\}\},$$

$$\theta(n, k) = \max_{A \in \Gamma(n, k)} f(A) \quad \text{and} \quad \Theta(n, k) = \{A \in \Gamma(n, k) : f(A) = \theta(n, k)\}.$$

Let  $A \in M_n\{0, 1\}$ ,  $B$  an  $m \times m$  principal submatrix of  $A$ , then it is clear that  $A \in \Gamma(n, k)$  implies  $B \in \Gamma(m, k)$ . Moreover, given any  $n \times n$  permutation matrix  $P$ ,  $A \in \Gamma(n, k)$  if and only if  $P^T A P \in \Gamma(n, k)$ .

To determine  $\theta(n, k)$  and  $\Theta(n, k)$  is an interesting problem posed by Zhan (see [15, page 234]), which has been partially solved by Wu [14], Huang and Zhan [8].

Given a digraph  $D$ , the  $(i, j)$ -entry of  $(A_D)^k$  equals  $t$  if and only if there are exactly  $t$  distinct directed walks of length  $k$  from vertex  $v_i$  to vertex  $v_j$  in  $D$ . Hence, a digraph  $D$  is  $\mathcal{F}_k$ -free if and only if its adjacency matrix  $A_D$  is in  $\Gamma(n, k)$ . Moreover,

$$\theta(n, k) = ex(n, \mathcal{F}_k). \quad (3.1)$$

It should be noticed that (3.1) is not necessarily true for strict digraphs.

For digraphs allowing loops, Huang and Zhan determined  $ex(n, \mathcal{F}_k)$  and  $Ex(n, \mathcal{F}_k)$  for  $k \geq n - 1 \geq 4$  as follows.

**Theorem 3** ([8]). *Let  $n, k$  be given integers such that  $k \geq n - 1 \geq 4$ . Then  $ex(n, \mathcal{F}_k) = n(n - 1)/2$  and a digraph  $D$  is in  $Ex(n, \mathcal{F}_k)$  if and only if  $D$  is a transitive tournament of order  $n$ .*

They also determine  $ex(n, \mathcal{F}_{n-2}) = n(n - 1)/2 - 1$  for  $n \geq 6$  and  $ex(n, \mathcal{F}_{n-3}) = n(n - 1)/2 - 2$  for  $n \geq 7$ . Hence, when  $k \geq 4$ ,  $ex(n, \mathcal{F}_k)$  for  $5 \leq n \leq k + 3$  and  $Ex(n, \mathcal{F}_k)$  for  $5 \leq n \leq k + 1$  have been determined.

In the following of this section, we will determine  $ex(k + 4, \mathcal{F}_k)$  and  $Ex(n, \mathcal{F}_k)$  for  $k \geq 4$  and  $n = k + 2, k + 3, k + 4$ . We need the following lemmas.

**Lemma 4.** *Let  $n \geq 3$ ,  $p$  and  $q$  be nonnegative integers such that  $(p, q) \neq (0, 0)$ , and let  $A \in M_n\{0, 1\}$ . If*

$$f(A(i)) \leq \frac{(n - 1)(n - 2)}{2} - p \frac{n - 1}{2} - q \text{ for all } 1 \leq i \leq n,$$

*then*

$$f(A) \leq \frac{n(n - 1)}{2} - p \frac{n + 1}{2} - q - 1. \quad (3.2)$$

*Proof.* Using the same idea as in the proof of [8, Corollary 10], we count the number of ones in the principal submatrices  $A(1), \dots, A(n)$ . Note that each diagonal entry of  $A$  appears  $n - 1$  times and each off-diagonal entry of  $A$  appears  $n - 2$  times in these submatrices. Suppose  $A$  has  $d$  nonzero diagonal entries. Then

$$(n - 1)d + (n - 2)[f(A) - d] = \sum_{i=1}^n f(A(i)) \leq n \left[ \frac{(n - 1)(n - 2)}{2} - p \frac{n - 1}{2} - q \right].$$

It follows that

$$f(A) \leq \frac{n(n-1)}{2} - p\frac{n+1}{2} - q - \frac{p+2q}{n-2} - \frac{d}{n-2}.$$

Since  $(p+2q)/(n-2) > 0$ ,  $d/(n-2) \geq 0$  and  $f(A)$  is an integer, we get (3.2).  $\square$

For the sake of convenience, we will always use  $\{1, 2, \dots, n\}$  to denote the vertex set of a digraph  $D$  of order  $n$  and use the notation  $i \rightarrow j$  to denote the arc  $(i, j)$ .

**Lemma 5.** *Let  $m = k + t + s + 1$  with  $s \geq 1$ ,  $k \geq 1$ ,  $t \geq 3$  being integers, and let  $x_1, y_1 \in \mathbb{R}^k$ ,  $x_2, y_2 \in \mathbb{R}^t$ ,  $x_3, y_3 \in \mathbb{R}^s$ . If*

$$(a_{ij}) = \begin{bmatrix} 0 & J_{k,t} & J_{k,s} & x_1 \\ 0 & T_t & J_{t,s} & x_2 \\ 0 & 0 & 0 & x_3 \\ y_1^T & y_2^T & y_3^T & \alpha \end{bmatrix} \in \Gamma(m, t+1)$$

and

$$\sum_{i=1}^3 [f(x_i) + f(y_i)] + \alpha \geq s + k + 2,$$

then

$$\alpha = 0, \quad y_1 = 0, \quad x_3 = 0, \quad \text{and } a_{im}a_{mj} = 0 \text{ for all } j \leq i+2, 1 \leq i, j \leq n.$$

*Proof.* Denote  $A = (a_{ij})$ . First we claim that  $x_3 = 0$  and  $y_1 = 0$ . Otherwise suppose  $x_3 \neq 0$  or  $y_1 \neq 0$ . Then  $a_{im} = 1$  for some  $i \in \{k+t+1, \dots, k+t+s\}$  or  $a_{mj} = 1$  for some  $j \in \{1, 2, \dots, k\}$ . It follows that  $D(A)$  has two distinct walks of length  $t+1$  from  $k$  to  $m$  or from  $m$  to  $k+t+1$ :

$$\begin{cases} k \rightarrow k+1 \rightarrow k+3 \rightarrow \dots \rightarrow k+t \rightarrow i \rightarrow m, \\ k \rightarrow k+2 \rightarrow k+3 \rightarrow \dots \rightarrow k+t \rightarrow i \rightarrow m, \end{cases}$$

$$\begin{cases} m \rightarrow j \rightarrow k+1 \rightarrow k+3 \rightarrow k+4 \rightarrow \dots \rightarrow k+t+1, \\ m \rightarrow j \rightarrow k+1 \rightarrow k+2 \rightarrow k+4 \rightarrow \dots \rightarrow k+t+1, \end{cases}$$

which contradicts  $A \in \Gamma(m, t+1)$ . Hence,  $x_3$  and  $y_1$  are zero vectors.

Next we assert that  $\alpha = 0$ . Otherwise,  $\alpha = 1$ . Since

$$\sum_{i=1}^3 (f(x_i) + f(y_i)) \geq s + k + 1,$$

we have either

$$\sum_{i=1}^3 f(x_i) \geq k+1 \text{ or } \sum_{i=1}^3 f(y_i) \geq s+1.$$

If  $\sum_{i=1}^3 f(x_i) \geq k+1$ , then the last column of  $A$  has at least two nonzero entries  $a_{im} = a_{jm} = 1$  with  $1 \leq i < j \leq k+t$ . Hence  $D(A)$  has the following two distinct walks of length  $t+1$  from  $i$  to  $m$ :

$$\begin{cases} i \rightarrow m \rightarrow m \rightarrow m \rightarrow \cdots \rightarrow m, \\ i \rightarrow j \rightarrow m \rightarrow m \rightarrow \cdots \rightarrow m. \end{cases}$$

If  $\sum_{i=1}^3 f(y_i) \geq s+1$ , then the last row of  $A$  has at least two nonzero entries  $a_{mi} = a_{mj} = 1$  with  $k+1 \leq i < j \leq m$  and  $i \leq k+t$ . It follows that  $D(A)$  has the following two distinct walks of length  $t+1$  from  $m$  to  $j$ :

$$\begin{cases} m \rightarrow m \rightarrow \cdots \rightarrow m \rightarrow i \rightarrow j, \\ m \rightarrow m \rightarrow \cdots \rightarrow m \rightarrow m \rightarrow j. \end{cases}$$

In both cases we get contradictions. Therefore,  $\alpha = 0$ .

Next we claim  $a_{im}a_{mj} = 0$  for  $j \leq i+2$ . Otherwise suppose  $a_{im} = a_{mj} = 1$  with  $1 \leq i, j \leq m-1$  and  $j \leq i+2$ . Since  $x_3 = y_1 = 0$ , we have  $i \leq k+t$  and  $j \geq k+1$ . We distinguish the following cases to find two distinct walks of length  $t+1$  with the same endpoints in  $D(A)$ , which contradicts  $A \in \Gamma(m, t+1)$ . If  $i \leq k$ , then  $j \leq k+2$  and  $D(A)$  has

$$\begin{cases} i \rightarrow k+1 \rightarrow k+2 \rightarrow \cdots \rightarrow k+t+1, \\ i \rightarrow m \rightarrow j \rightarrow k+3 \rightarrow \cdots \rightarrow k+t+1. \end{cases}$$

If  $k < i \leq k+t-2$ , then  $j \leq k+t$  and  $D(A)$  has

$$\begin{cases} k \rightarrow k+1 \rightarrow k+2 \rightarrow \cdots \rightarrow k+t \rightarrow k+t+1, \\ k \rightarrow k+1 \rightarrow \cdots \rightarrow i \rightarrow m \rightarrow j \rightarrow i+3 \rightarrow \cdots \rightarrow k+t+1. \end{cases}$$

If  $i = k+t-1$ , then  $j \leq k+t+1$  and  $D(A)$  has

$$\begin{cases} k \rightarrow k+1 \rightarrow k+2 \rightarrow \cdots \rightarrow i \rightarrow k+t \rightarrow k+t+1, \\ k \rightarrow k+1 \rightarrow k+2 \rightarrow \cdots \rightarrow i \rightarrow m \rightarrow k+t+1, \text{ if } j = k+t+1, \\ k \rightarrow k+2 \rightarrow \cdots \rightarrow i \rightarrow m \rightarrow j \rightarrow \cdots \rightarrow k+t+1, \text{ if } j \leq k+t. \end{cases}$$

If  $i = k+t$ , then  $j \leq k+t+2$  and  $D(A)$  has

$$\begin{cases} k \rightarrow k+2 \rightarrow k+3 \rightarrow \cdots \rightarrow i \rightarrow m \rightarrow j, \\ k \rightarrow k+1 \rightarrow k+3 \rightarrow \cdots \rightarrow i \rightarrow m \rightarrow j. \end{cases}$$

Therefore,  $a_{im}a_{mj} = 0$  for all  $j \leq i+2$ . □

**Corollary 6.** Let  $x, y \in \mathbb{R}^{n-1}$  with  $n \geq 6$ . If

$$\begin{bmatrix} T_{n-1} & x \\ y^T & \beta \end{bmatrix} \in \Gamma(n, n-2), \quad (3.3)$$

and

$$f(x) + f(y) + \beta = n-2,$$

then one of the following holds:

(1)  $x = (1, \dots, 1, 0)^T, y = 0$  and  $\beta = 0$ ;

(2)  $y = (0, 1, \dots, 1)^T, x = 0$  and  $\beta = 0$ .

*Proof.* Denote the matrix in (3.3) by  $A = (a_{ij})$ . Applying Lemma 5 with  $k = s = 1$ , we have

$$\beta = a_{n1} = a_{n-1,n} = 0, \text{ and } a_{in}a_{nj} = 0 \text{ for all } j \leq i + 2. \quad (3.4)$$

We assert  $f(x) = 0$  or  $f(y) = 0$ . Otherwise, assume that  $a_{i_0n}$  is the last nonzero component in  $x$ , and  $a_{nj_0}$  is the first nonzero component in  $y$ . Since  $f(x) + f(y) = n - 2 \leq i_0 + n - 1 - (j_0 - 1)$ , we have  $j_0 - i_0 \leq 2$ , and  $a_{i_0n}a_{nj_0} = 0$  follows from (3.4), which contradicts the assumption that  $a_{i_0n}a_{nj_0} = 1$ . Therefore,  $x = 0$  or  $y = 0$ . It follows that either (1) or (2) holds.  $\square$

Now we are ready to characterize  $Ex(k + 2, \mathcal{F}_k)$  and  $Ex(k + 3, \mathcal{F}_k)$  for  $k \geq 4$ .

**Theorem 7.** *Let  $n \geq 6$  be an integer. Then*

$$ex(n, \mathcal{F}_{n-2}) = \frac{n(n-1)}{2} - 1. \quad (3.5)$$

Moreover, a digraph  $D$  is in  $Ex(n, \mathcal{F}_{n-2})$  if and only if  $A_D$  is permutation similar to

$$K_n \equiv \begin{bmatrix} T_{n-2} & J_{n-2,2} \\ 0 & 0 \end{bmatrix} \quad \text{or} \quad K'_n \equiv \begin{bmatrix} 0 & J_{2,n-2} \\ 0 & T_{n-2} \end{bmatrix}.$$

*Proof.* By [8, Corollary 10] we get (3.5). Suppose  $D$  is a digraph in  $Ex(n, \mathcal{F}_{n-2})$  and  $A \equiv A_D$ . Applying Lemma 4, there exists some  $i \in \{1, 2, \dots, n\}$  such that  $f(A(i)) \geq \frac{(n-1)(n-2)}{2}$ . Since  $A(i) \in \Gamma(n-1, n-2)$ , applying Theorem 3 we get  $f(A(i)) = \frac{(n-1)(n-2)}{2}$  and  $A(i)$  is permutation similar to  $T_{n-1}$ . Using permutation similarity if necessary, without loss of generality we assume  $i = n$  and

$$A = \begin{bmatrix} T_{n-1} & x \\ y^T & \alpha \end{bmatrix}$$

with  $x, y \in \mathbb{R}^{n-1}$ . It follows that

$$f(x) + f(y) + \alpha = f(A) - f(A(n)) = ex(n, \mathcal{F}_{n-2}) - \frac{(n-1)(n-2)}{2} = n - 2.$$

Applying Corollary 6, one of the following holds.

(1)  $x = (1, \dots, 1, 0)^T, y = 0$  and  $\alpha = 0$ . Then  $A = K_n$ ;



(2)  $y = (0, 1, \dots, 1)^T$ ,  $x = 0$  and  $\alpha = 0$ . Then  $PAP^T = K'_n$ , where

$$P = \begin{bmatrix} 0 & 1 \\ I_{n-1} & 0 \end{bmatrix}.$$

Therefore,  $A_D$  is permutation similar to  $K_n$  or  $K'_n$ .

Conversely, if the adjacency matrix  $A$  of a digraph  $D$  is permutation similar to  $K_n$  or  $K'_n$ , by direct computation we can verify  $f(A) = ex(n, \mathcal{F}_{n-2})$  and  $A^{n-2} \in M_n\{0, 1\}$ . Hence  $D \in Ex(n, \mathcal{F}_{n-2})$ .  $\square$

**Theorem 8.** *Let  $n \geq 7$  be an integer. Then*

$$ex(n, \mathcal{F}_{n-3}) = \frac{n(n-1)}{2} - 2. \quad (3.6)$$

Moreover, a digraph  $D$  is in  $Ex(n, \mathcal{F}_{n-3})$  if and only if  $A_D$  is permutation similar to

$$F_n \equiv \begin{bmatrix} 0 & J_{2,n-4} & J_{2,2} \\ 0 & T_{n-4} & J_{n-4,2} \\ 0 & 0 & 0 \end{bmatrix}.$$

*Proof.* From [8, Corollary 11] we get (3.6). Suppose  $D \in Ex(n, \mathcal{F}_{n-3})$  and  $A \equiv A_D$ . Applying 4 we see that  $A$  contains a submatrix  $A(i)$ , say  $A(n)$ , such that  $f(A(n)) \geq \frac{(n-1)(n-2)}{2} - 1$ . By Theorem 7,  $f(A(n)) = \frac{(n-1)(n-2)}{2} - 1$  and  $A(n)$  is permutation similar to  $K_{n-1}$  or  $K'_{n-1}$ .

First we consider the case that  $A(n)$  is permutation similar to  $K_{n-1}$ . Without loss of generality we can assume  $A(n) = K_{n-1}$  and

$$A = \begin{bmatrix} 0 & J_{1,n-4} & J_{1,2} & x_1 \\ 0 & T_{n-4} & J_{n-4,2} & x_2 \\ 0 & 0 & 0 & x_3 \\ y_1^T & y_2^T & y_3^T & \alpha \end{bmatrix},$$

where  $x_1, y_1 \in \mathbb{R}$ ,  $x_2, y_2 \in \mathbb{R}^{n-4}$ , and  $x_3, y_3 \in \mathbb{R}^2$ .

Let  $x = (x_1^T, x_2^T, x_3^T)$  and  $y = (y_1^T, y_2^T, y_3^T)$ . Then

$$\alpha + f(x) + f(y) = f(A) - f(A(n)) = n - 2.$$

Applying Lemma 5, we get  $x_3 = 0$ , i.e.,  $a_{n-2,n} = a_{n-1,n} = 0$ .

Let  $i = n - 2$  or  $n - 1$ . Then

$$f(A(i)) = f(A) - (n - 3) - a_{ni} = \frac{(n-1)(n-2)}{2} - a_{ni}. \quad (3.7)$$

On the other hand, since  $A(i) \in \Gamma(n-1, n-3)$ , by Theorem 7 we have

$$f(A(i)) \leq \frac{(n-1)(n-2)}{2} - 1. \quad (3.8)$$

Combining (3.7) and (3.8) we get  $a_{ni} = 1$ .

Now applying Corollary 6 to  $A(n-1)$  we have  $y = (0, 1, \dots, 1)$ ,  $x = 0$ ,  $\alpha = 0$ , and

$$A = \begin{bmatrix} 0 & J_{1,n-4} & J_{1,2} & 0 \\ 0 & T_{n-4} & J_{n-4,2} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & J_{1,n-4} & J_{1,2} & 0 \end{bmatrix} = P^T F_n P$$

where

$$P = \begin{bmatrix} 0 & 1 \\ I_{n-1} & 0 \end{bmatrix}.$$

Next suppose  $A(n)$  is permutation similar to  $K'_{n-1}$ . Without loss of generality we can assume  $A(n) = K'_{n-1}$  and

$$A = \begin{bmatrix} 0 & J_{2,n-4} & J_{2,1} & x_1 \\ 0 & T_{n-4} & J_{n-4,1} & x_2 \\ 0 & 0 & 0 & x_3 \\ y_1^T & y_2^T & y_3^T & \alpha \end{bmatrix},$$

where  $x_1, y_1 \in \mathbb{R}^2$ ,  $x_2, y_2 \in \mathbb{R}^{n-4}$ , and  $x_3, y_3 \in \mathbb{R}$ . Applying the same argument as above by counting  $f(A(1))$ ,  $f(A(2))$  and applying Corollary 6 to  $A(1)$ , we get  $A = F_n$ .

Conversely, if the adjacency matrix  $A$  of a digraph  $D$  is permutation similar to  $F_n$ , by direct computation we can verify  $f(A) = ex(n, \mathcal{F}_{n-3})$  and  $A^{n-3} \in M_n\{0, 1\}$ . Hence  $D \in Ex(n, \mathcal{F}_{n-3})$ . □

Next we determine  $ex(k+4, \mathcal{F}_k)$  for  $k \geq 4$  and  $Ex(k+4, \mathcal{F}_k)$  for  $k \geq 5$ .

**Lemma 9.** *Let  $x, y \in \mathbb{R}^{n-1}$  with  $n \geq 6$ , and*

$$A = \begin{bmatrix} T_{n-1} & x \\ y^T & \alpha \end{bmatrix}.$$

(i) *If  $f(x) + f(y) + \alpha = n - 2$ , then  $A \in \Gamma(n, n - 1)$  if and only if*

$$\alpha = 0, \quad x = (a^T, 0)^T, \quad y = (0, b^T)^T, \quad (3.9)$$

*where  $a \in \mathbb{R}^s$ ,  $b \in \mathbb{R}^{n-s-1}$  with  $s \in \{0, 1, \dots, n-2\}$ . Here  $s = 0$  means  $x = 0$ .*

(ii) *If  $f(x) + f(y) + \alpha = n - 1$ , then  $A \in \Gamma(n, n - 1)$  if and only if*

$$\alpha = 0, \quad x = (J_{1,s}, 0)^T, \quad y = (0, J_{1,n-s-1})^T, \quad (3.10)$$

*where  $s \in \{0, 1, \dots, n-2\}$ .*

*Proof.* (i) Suppose  $A \in \Gamma(n, n-1)$ . First we claim  $\alpha = 0$ . Otherwise, since  $f(x) + f(y) = n-3 \geq 3$ , we have either  $f(x) \geq 2$  or  $f(y) \geq 2$ . If  $f(x) \geq 2$ , say,  $a_{in} = a_{jn} = 1$  with  $1 \leq i < j \leq n-1$ , then  $D(A)$  has the following two distinct walks from  $i$  to  $n$  with the same length  $n-1$ :

$$\begin{cases} i \rightarrow n \rightarrow n \rightarrow n \rightarrow \cdots \rightarrow n, \\ i \rightarrow j \rightarrow n \rightarrow n \rightarrow \cdots \rightarrow n. \end{cases}$$

If  $f(y) \geq 2$ , say,  $a_{ni} = a_{nj} = 1$  with  $1 \leq i < j \leq n-1$ , then  $D(A)$  has the following two distinct walks from  $n$  to  $j$  with the same length  $n-1$ :

$$\begin{cases} n \rightarrow n \rightarrow \cdots \rightarrow n \rightarrow i \rightarrow j, \\ n \rightarrow n \rightarrow \cdots \rightarrow n \rightarrow n \rightarrow j. \end{cases}$$

In both cases we get contradictions. Hence  $\alpha = 0$ .

Next we claim

$$a_{in}a_{nj} = 0 \quad \text{for all } i \geq j. \quad (3.11)$$

If  $x = 0$  or  $y = 0$ , the claim is clear. Suppose  $x, y$  are nonzero, and there exist  $i \geq j$  such that  $a_{in}a_{nj} = 1$ . Then we have the following cases and in each of these cases  $D(A)$  has two different walks of length  $n-1$  with the same endpoints, which contradicts  $A \in \Gamma(n, n-1)$ .

*Case 1.*  $i \leq 2$ .  $D(A)$  has

$$\begin{cases} 1 \rightarrow i \rightarrow n \rightarrow j \rightarrow i+2 \rightarrow i+3 \rightarrow \cdots \rightarrow n-1, \\ 1 \rightarrow i \rightarrow n \rightarrow j \rightarrow i+1 \rightarrow i+3 \rightarrow \cdots \rightarrow n-1, \end{cases}$$

where the arc  $1 \rightarrow i$  does not appear if  $i = 1$ .

*Case 2.*  $i = 3$ .  $D(A)$  has

$$\begin{cases} 1 \rightarrow 3 \rightarrow n \rightarrow j \rightarrow i+1 \rightarrow \cdots \rightarrow n-1, \\ 1 \rightarrow 2 \rightarrow 3 \rightarrow n \rightarrow j \rightarrow i+2 \rightarrow \cdots \rightarrow n-1. \end{cases}$$

*Case 3.*  $4 \leq i \leq n-1$ .  $D(A)$  has

$$\begin{cases} 1 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \rightarrow i \rightarrow n \rightarrow j \rightarrow i+1 \rightarrow \cdots \rightarrow n-1, \\ 1 \rightarrow 2 \rightarrow 4 \rightarrow \cdots \rightarrow i \rightarrow n \rightarrow j \rightarrow i+1 \rightarrow \cdots \rightarrow n-1, \end{cases}$$

where the walk  $j \rightarrow i+1 \rightarrow \cdots \rightarrow n-1$  does not appear if  $i = n-1$ .

Let  $a_{sn}$  be the last nonzero component in  $x$  and  $a_{nt}$  be the first nonzero component in  $y$ . Since  $f(x) + f(y) = n-2$ , by (3.11) we have  $t-s = 1$  or  $2$ . Hence (3.9) holds.

Conversely, suppose  $A$  satisfies (3.9). Let

$$B = \begin{bmatrix} T_s & J_{s,n-s-1} & J_{s,1} \\ 0 & T_{n-s-1} & 0 \\ 0 & J_{1,n-s-1} & 0 \end{bmatrix}$$

with  $0 \leq s \leq n-1$ . To prove  $A \in \Gamma(n, n-1)$ , it suffices to verify  $B \in \Gamma(n, n-1)$ , since  $B \geq A$ , where the notation  $\geq$  is to be understood entrywise.

If  $s = n-1$ , then  $B = T_n \in \Gamma(n, n-1)$ . If  $s < n-1$ , then

$$B = \begin{bmatrix} T_s & J_{s,1} & J_{s,n-s-2} & J_{s,1} \\ 0 & 0 & J_{1,n-s-2} & 0 \\ 0 & 0 & T_{n-s-2} & 0 \\ 0 & 1 & J_{1,n-s-2} & 0 \end{bmatrix}$$

is permutation similar to

$$\begin{bmatrix} T_s & J_{s,1} & J_{s,1} & J_{s,n-s-2} \\ 0 & 0 & 1 & J_{1,n-s-2} \\ 0 & 0 & 0 & J_{1,n-s-2} \\ 0 & 0 & 0 & T_{n-s-2} \end{bmatrix} = T_n.$$

Therefore,  $B \in \Gamma(n, n-1)$ . This completes the proof for (i).

(ii) For the sufficiency part, if (3.10) holds, then  $A = B \in \Gamma(n, n-1)$ . For the necessity part, let  $a_{sn}$  be the last nonzero component in  $x$  and  $a_{nt}$  be the first nonzero component in  $y$ . Since  $f(x) + f(y) = n-1$ , applying the same arguments as above we get  $\alpha = 0$  and  $t-s = 1$ . It follows that (3.10) holds.  $\square$

**Theorem 10.** *Let  $n \geq 8$  be an integer. Then*

$$ex(n, \mathcal{F}_{n-4}) = \frac{n(n-1)}{2} - 4. \quad (3.12)$$

*Proof.* Let  $A$  be the adjacency matrix of any  $\mathcal{F}_{n-4}$ -free digraph  $D$  of order  $n$ . Then  $A \in \Gamma(n, n-4)$  and  $A(i) \in \Gamma(n-1, n-4)$  for all  $1 \leq i \leq n$ . Hence

$$f(A(i)) \leq ex(n-1, \mathcal{F}_{n-4}) = \frac{(n-1)(n-2)}{2} - 2$$

for all  $1 \leq i \leq n$ . By Lemma 4, we have

$$f(A) \leq \frac{n(n-1)}{2} - 3. \quad (3.13)$$

Suppose equality in (3.13) holds. Then by Lemma 4,  $A$  contains a submatrix  $A(i)$  with  $\frac{(n-1)(n-2)}{2} - 2$  nonzero entries. Using permutation similarity if necessary, without loss of generality we assume  $f(A(n)) = \frac{(n-1)(n-2)}{2} - 2$ . Since  $A(n) \in \Gamma(n-1, n-4)$ , by Theorem 8, we may further assume

$$A = (a_{ij}) = \begin{bmatrix} 0 & J_{2,n-5} & J_{2,2} & x_1 \\ 0 & T_{n-5} & J_{n-5,2} & x_2 \\ 0 & 0 & 0 & x_3 \\ y_1^T & y_2^T & y_3^T & \alpha \end{bmatrix}, \quad (3.14)$$

where  $x_1, x_3, y_1, y_3 \in \mathbb{R}^2$ ,  $x_2, y_2 \in \mathbb{R}^{n-5}$ .

Let  $x = (x_1^T, x_2^T, x_3^T)$  and  $y = (y_1^T, y_2^T, y_3^T)$ . Then

$$f(x) + f(y) + \alpha = f(A) - f(A(n)) = n - 2.$$

Applying Lemma 5 to  $A$  we know  $y_1 = x_3 = 0$  and  $\alpha = 0$ .

Since  $a_{n-1,n} = a_{n1} = 0$  and  $A(1, n-1) \in \Gamma(n-2, n-4)$ , by (3.14) we have

$$\begin{aligned} f(A(1, n-1)) &= f(A) - 2(n-5) - 3 - a_{1n} - a_{n1} - a_{n-1,n} - a_{n,n-1} \\ &= \frac{(n-2)(n-3)}{2} + 1 - a_{1n} - a_{n,n-1} \\ &\leq \frac{(n-2)(n-3)}{2} - 1 \end{aligned}$$

where the inequality follows from Theorem 7. Hence,

$$a_{1n} = a_{n,n-1} = 1. \quad (3.15)$$

On the other hand, applying Corollary 6 to  $A(1, n-1)$  we have either  $x = 0$  or  $y = 0$ , which contradicts (3.15). Hence, (3.13) is a strict inequality and we have

$$ex(n, \mathcal{F}_{n-4}) \leq \frac{n(n-1)}{2} - 4. \quad (3.16)$$

Now let  $D$  be the digraph with adjacency matrix

$$B = \begin{bmatrix} 0 & J_{3,n-5} & J_{3,2} \\ 0 & T_{n-5} & J_{n-5,2} \\ 0 & 0 & 0 \end{bmatrix}.$$

By direct computation, we have

$$B^{n-4} = \begin{bmatrix} 0 & 0 & J_{3,2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and hence  $D$  is  $\mathcal{F}_{n-4}$ -free. Therefore,

$$ex(n, \mathcal{F}_{n-4}) \geq f(B) = \frac{n(n-1)}{2} - 4. \quad (3.17)$$

Combining (3.16) and (3.17) we get (3.12).  $\square$

**Lemma 11.** Let  $k \geq 5$  and  $s$  be positive integers, let  $x_i, y_i \in \mathbb{R}^k$  with components from  $\{0, 1\}$  for  $i = 1, 2, \dots, s$ , and let

$$A = (a_{ij}) = \begin{bmatrix} T_k & x_1 & x_2 & x_3 & \cdots & x_s \\ y_1^T & 0 & 1 & 0 & \cdots & 0 \\ y_2^T & 0 & 0 & 1 & \ddots & \vdots \\ y_3^T & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ y_s^T & 1 & 0 & \cdots & \cdots & 0 \end{bmatrix}$$

- (i) If there is some  $i \in \{1, 2, \dots, s\}$  such that  $f(x_i) \geq 3$  or  $f(y_i) \geq 3$ , then  $A \notin \Gamma(k+s, p)$  for any integer  $p \geq 2$ .
- (ii) If  $s = 2$  and there is some  $i \in \{1, 2\}$  such that  $f(x_i) = f(y_i) = 2$ , then  $A \notin \Gamma(k+s, p)$  for any integer  $p \geq 5$ .

*Proof.* (i) If there is some  $t$  such that  $f(x_t) \geq 3$ , then we have  $a_{i,k+t} = a_{j,k+t} = a_{m,k+t} = 1$  for  $1 \leq i < j < m \leq k$ . Without loss of generality we assume  $t = 1$ . For any  $p \in \{2, 3, \dots, k\}$ , we can find two distinct walks of length  $p$  between the same endpoints in the following walks in  $D(A)$ .

$$\begin{cases} i \rightarrow j \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+s \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \\ i \rightarrow m \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+s \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \end{cases}$$

If there is some  $t$ , say  $t = 1$ , such that  $f(y_t) \geq 3$ , then we have  $a_{k+1,i} = a_{k+1,j} = a_{k+1,m} = 1$  for  $1 \leq i < j < m \leq k$ . For any  $p \in \{2, 3, \dots, k\}$ , we can find two distinct walks of length  $p$  between the same endpoints in the following walks in  $D(A)$

$$\begin{cases} \dots \rightarrow k+s \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+s \rightarrow k+1 \rightarrow i \rightarrow m, \\ \dots \rightarrow k+s \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+s \rightarrow k+1 \rightarrow j \rightarrow m. \end{cases}$$

Therefore,  $A \notin \Gamma(k+s, p)$  for any  $p \in \{2, 3, \dots, k\}$ .

(ii) Without loss of generality, we assume  $f(x_1) = f(y_1) = 2$  and  $a_{p_1,k+1} = a_{p_2,k+1} = a_{k+1,q_1} = a_{k+1,q_2} = 1$  with  $1 \leq p_1 < p_2 \leq k$  and  $1 \leq q_1 < q_2 \leq k$ . If  $p \geq 5$  is odd, then  $D(A)$  has the following two distinct walks of length  $p$  from  $p_1$  to  $q_2$ :

$$\begin{cases} p_1 \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+1 \rightarrow q_1 \rightarrow q_2, \\ p_1 \rightarrow p_2 \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+1 \rightarrow q_2. \end{cases}$$

If  $p \geq 5$  is even, then  $D(A)$  has the following two distinct walks of length  $p$  from  $p_1$  to  $q_2$ :

$$\begin{cases} p_1 \rightarrow p_2 \rightarrow k+1 \rightarrow k+2 \rightarrow \dots \rightarrow k+1 \rightarrow q_1 \rightarrow q_2, \\ p_1 \rightarrow k+1 \rightarrow k+2 \rightarrow k+1 \rightarrow \dots \rightarrow k+2 \rightarrow k+1 \rightarrow q_2. \end{cases}$$

Therefore,  $A \notin \Gamma(k+s, p)$  for any integer  $p \geq 5$ . □

**Theorem 12.** Let  $n \geq 9$  be an integer. Then a digraph  $D$  is in  $Ex(n, \mathcal{F}_{n-4})$  if and only if  $A_D$  is permutation similar to one of the following matrices

$$F_1(n) \equiv \begin{bmatrix} 0 & J_{3,n-5} & J_{3,2} \\ 0 & T_{n-5} & J_{n-5,2} \\ 0 & 0 & 0 \end{bmatrix}, \quad F_2(n) \equiv \begin{bmatrix} 0 & J_{2,n-5} & J_{2,3} \\ 0 & T_{n-5} & J_{n-5,3} \\ 0 & 0 & 0 \end{bmatrix},$$

$$F_3(n) \equiv \begin{bmatrix} 0 & J_{2,n-5} & J_{2,2} & J_{2,1} \\ 0 & T_{n-5} & J_{n-5,2} & U_m \\ 0 & 0 & 0 & 0 \\ 0 & U'_m & J_{1,2} & 0 \end{bmatrix}, \quad F_4(n) \equiv \begin{bmatrix} T_{n-4} & w_1 & w_2 & w_3 & w_4 \\ u_1 & 0 & 1 & 1 & 1 \\ u_2 & 0 & 0 & 1 & 1 \\ u_3 & 0 & 0 & 0 & 1 \\ u_4 & 0 & 0 & 0 & 0 \end{bmatrix},$$

where

$$U_m = (J_{1,m}, 0)^T, \quad U'_m = (0, J_{1,n-m-7}) \quad \text{with } 0 \leq m \leq n-7$$

and

$$w_j = (J_{1,k_j}, 0)^T, \quad u_j = (0, J_{1,n-k_j-5}) \quad \text{for } i = 1, 2, 3, 4$$

with  $0 \leq k_1 < k_2 < k_3 < k_4 \leq n-5$ .

*Proof.* Suppose  $A \equiv A_D$  is permutation similar to one of  $F_1(n), F_2(n), F_3(n)$  and  $F_4(n)$ . It is clear that  $f(A) = \frac{n(n-1)}{2} - 4$ . To prove  $D \in Ex(n, \mathcal{F}_{n-4})$ , it suffices to prove  $F_i^{n-4}(n) \in M_n\{0, 1\}$  for  $i = 1, 2, 3, 4$ .

By direct computation we know

$$F_1^{n-4}(n) = \begin{bmatrix} 0 & J_{3,2} \\ 0 & 0 \end{bmatrix}, \quad F_2^{n-4}(n) = \begin{bmatrix} 0 & J_{2,3} \\ 0 & 0 \end{bmatrix}, \quad F_3^{n-4}(n) = \begin{bmatrix} 0 & J_{2,2} & O_{2 \times 1} \\ 0 & 0 & 0 \end{bmatrix}$$

are all 0-1 matrices, where  $O_{2 \times 1}$  is the  $2 \times 1$  zero matrix.

For  $i = 4$ , let  $\alpha = \{1, 2, \dots, n-4, n-3+k_1, n-3+k_2, n-3+k_3, n-3+k_4\}$  and

$$A' \equiv J_2 \otimes T_{n-4} = \begin{bmatrix} T_{n-4} & T_{n-4} \\ T_{n-4} & T_{n-4} \end{bmatrix}.$$

Then  $F_4(n) = A'[\alpha]$  is a principal submatrix of  $A'$ . Moreover,

$$(A')^{n-4} = (J_2 \otimes T_{n-4})^{n-4} = J_2^{n-4} \otimes T_{n-4}^{n-4} = 0$$

implies  $F_4^{n-4}(n) = 0$ . Thus we get the sufficiency of Theorem 12.

Next we prove the necessity part of Theorem 12. Suppose  $D \in Ex(n, \mathcal{F}_{n-4})$ . Denote by  $A \equiv A_D$  the adjacency matrix of  $D$ . Then  $f(A) = ex(n, \mathcal{F}_{n-4})$ ,  $A \in \Gamma(n, n-4)$  and  $A(i) \in \Gamma(n-1, n-4)$  for all  $1 \leq i \leq n$ . By (3.6) we have

$$f(A(i)) \leq \frac{(n-1)(n-2)}{2} - 2 \quad \text{for all } 1 \leq i \leq n.$$

We distinguish two cases.

*Case 1.*  $f(A(q)) = \frac{(n-1)(n-2)}{2} - 2$  for some  $q \in \{1, 2, \dots, n\}$ . By Theorem 8, without loss of generality, we assume  $q = n$  and

$$A = \begin{bmatrix} 0 & J_{2,n-5} & J_{2,2} & x_1 \\ 0 & T_{n-5} & J_{n-5,2} & x_2 \\ 0 & 0 & 0 & x_3 \\ y_1^T & y_2^T & y_3^T & \alpha \end{bmatrix},$$

where  $x_1, x_3, y_1, y_3 \in \mathbb{R}^2$ ,  $x_2, y_2 \in \mathbb{R}^{n-5}$ . Let  $x = (x_1^T, x_2^T, x_3^T)$  and  $y = (y_1^T, y_2^T, y_3^T)$ . Since

$$f(x) + f(y) + \alpha = f(A) - f(A(n)) = n - 3 \geq 6, \quad (3.18)$$

applying Lemma 5, we have

$$\alpha = 0, \quad y_1 = x_3 = 0, \quad \text{and} \quad a_{in}a_{nj} = 0 \quad \text{for} \quad j \leq i + 2. \quad (3.19)$$

If  $x = 0$ , then  $A$  is permutation similar to  $F_1(n)$ . If  $y = 0$ , then  $A = F_2(n)$ . If both  $x$  and  $y$  are nonzero, let  $a_{sn}$  be the last nonzero component in  $x$  and  $a_{nt}$  be the first nonzero component in  $y$ . By (3.18) and (3.19) we have

$$t - s = 3, \quad x = (J_{1,s}, 0) \quad \text{and} \quad y = (0, J_{1,n-s-3}). \quad (3.20)$$

By exchanging row 1 and row 2 of  $A$ , and exchanging column 1 and column 2 of  $A$  simultaneously, we obtain a new matrix  $A' = (a'_{ij})$ . Applying Lemma 5 to  $A'$  we have  $a'_{in}a'_{nj} = 0$  for  $j \leq i + 2$ . Hence

$$a_{1n}a_{n4} = a'_{2n}a'_{n4} = 0.$$

Similarly, by interchanging the roles of the indices  $n - 1$  and  $n - 2$ , we get

$$a_{n-4,n}a_{n,n-1} = 0.$$

Therefore, in (3.20) we have  $s \neq 1$  and  $t \neq n - 1$ . Hence  $A = F_3(n)$  with  $m = s - 2$ .

Case 2.  $f(A(i)) \leq \frac{(n-1)(n-2)}{2} - 3$  for all  $i$ . Denote by

$$\delta_i = \sum_{j=1}^n a_{ij} + \sum_{j \neq i} a_{ji}$$

the number of nonzero entries in the  $i$ -th row and the  $i$ -th column of  $A$ . Then

$$\delta_i = f(A) - f(A(i)) \geq n - 2 \quad \text{for all} \quad 1 \leq i \leq n. \quad (3.21)$$

Applying Lemma 4 to  $A$ , there exists some  $i_0$  such that

$$f(A(i_0)) = \frac{(n-1)(n-2)}{2} - 3.$$

Without loss of generality, we assume  $i_0 = n$ . For any  $i \in \{1, \dots, n-1\}$ , since  $A(i, n) \in \Gamma(n-2, n-4)$ , by Theorem 7 we have

$$f(A(i, n)) \leq \frac{(n-2)(n-3)}{2} - 1. \quad (3.22)$$

Next we prove the following claim.



**Claim 1.** *Let  $i \in \{1, 2, \dots, n-1\}$ . Then*

$$f(A(i, n)) \leq \frac{(n-2)(n-3)}{2} - 2. \quad (3.23)$$

Moreover, there exists some  $i \in \{1, 2, \dots, n-1\}$  such that equality holds in (3.23).

Suppose equality in (3.22) holds for some  $i_1$ , say,  $i_1 = n-1$ . Then by Theorem 7,  $A(n-1, n)$  is permutation similar to  $K_{n-2}$  or  $K'_{n-2}$ . By (3.21) we have

$$\begin{aligned} \delta_{n-1} &= f(A(n)) - f(A(n-1, n)) + a_{n-1, n} + a_{n, n-1} \\ &= n - 4 + a_{n-1, n} + a_{n, n-1} \\ &\geq n - 2. \end{aligned}$$

It follows that  $a_{n-1, n} = a_{n, n-1} = 1$ .

If  $A(n-1, n)$  is permutation similar to  $K'_{n-2}$ , without loss of generality, we may assume

$$A = \begin{bmatrix} 0 & J_{2, n-4} & x_1 & x_3 \\ 0 & T_{n-4} & x_2 & x_4 \\ y_1^T & y_2^T & \alpha & 1 \\ y_3^T & y_4^T & 1 & \alpha' \end{bmatrix},$$

where  $x_1, x_3, y_1, y_3 \in \mathbb{R}^2$ ,  $x_2, y_2, x_4, y_4 \in \mathbb{R}^{n-4}$ . By [8, Lemma 1], we have  $\alpha = \alpha' = 0$  and

$$a_{in} + a_{ni} \leq 1 \quad \text{for all } 1 \leq i \leq n-2.$$

Thus  $f(x_3) + f(y_3) \leq 2$  and

$$f(x_3) + f(x_4) + f(y_3) + f(y_4) = \delta_n - 2 = n - 4 \geq 5. \quad (3.24)$$

If  $x_4$  has two nonzero entries, say,  $a_{i_1, n} = a_{i_2, n} = 1$  with  $3 \leq i_1, i_2 \leq n-2$ , then  $D$  has the following distinct walks of length  $n-4$  between the same endpoints

$$\begin{cases} 2 \rightarrow i_1 \rightarrow n \rightarrow n-1 \rightarrow n \rightarrow \dots \rightarrow n(\rightarrow n-1), \\ 2 \rightarrow i_2 \rightarrow n \rightarrow n-1 \rightarrow n \rightarrow \dots \rightarrow n(\rightarrow n-1). \end{cases}$$

Hence  $f(x_4) \leq 1$  and

$$f(y_4) = n - 4 - f(x_3) - f(y_3) - f(x_4) \geq n - 7 \geq 2. \quad (3.25)$$

If  $y_3$  and  $y_4$  have three nonzero entries, say,  $a_{n, j_1} = a_{n, j_2} = a_{n, j_3} = 1$  with  $j_1 < j_2 < j_3 \leq n-2$  and  $j_2 \geq 3$ , then  $D$  has the following distinct walks of length  $n-4$  between the same endpoints

$$\begin{cases} (n-1 \rightarrow) n \rightarrow n-1 \rightarrow n \rightarrow \dots \rightarrow n \rightarrow n-1 \rightarrow n \rightarrow j_3, \\ (n-1 \rightarrow) n \rightarrow n-1 \rightarrow n \rightarrow \dots \rightarrow n \rightarrow j_1 \rightarrow j_2 \rightarrow j_3. \end{cases}$$

Combining this with (3.24) and (3.25), we have

$$f(y_4) = 2, \quad y_3 = 0, \quad f(x_3) = 2 \quad \text{and} \quad f(x_4) = 1.$$

Suppose the nonzero entries in  $y_4$  are  $a_{n,j_1}$  and  $a_{n,j_2}$  with  $3 \leq j_1 < j_2 \leq n-2$ . Then  $D$  has two distinct walks of length  $n-4$  between the same endpoints in the following walks:

$$\begin{cases} 1 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \rightarrow n-2, \\ 1 \rightarrow n \rightarrow n-1 \rightarrow n \rightarrow \cdots \rightarrow n \rightarrow j_2 \rightarrow n-2, \\ 1 \rightarrow n \rightarrow n-1 \rightarrow n \rightarrow \cdots \rightarrow n \rightarrow j_1 \rightarrow j_2 \rightarrow n-2, \end{cases}$$

where  $j_2 \rightarrow n-2$  does not appear when  $j_2 = n-2$ . This contradicts the condition that  $A \in \Gamma(n, n-4)$ .

If  $A(n-1, n)$  is permutation similar to  $K_{n-2}$ , then we may assume

$$A = \begin{bmatrix} T_{n-4} & J_{n-4,2} & y_2 & y_4 \\ 0 & 0 & y_1 & y_3 \\ x_2^T & x_1^T & \alpha & 1 \\ x_4^T & x_3^T & 1 & \alpha' \end{bmatrix},$$

where  $x_1, x_3, y_1, y_3 \in \mathbb{R}^2$ ,  $x_2, y_2, x_4, y_4 \in \mathbb{R}^{n-4}$ . Applying similar arguments as above we can deduce  $A \notin \Gamma(n, n-4)$ , which contradicts  $D \in Ex(n, \mathcal{F}_{n-4})$ . Hence (3.22) is a strict inequality and we get (3.23).

On the other hand, applying Lemma 4 to  $A(n)$ , there exists some  $i \in \{1, 2, \dots, n-1\}$  such that equality in (3.23) holds. Thus we get Claim 1.

Now without loss of generality we assume  $f(A(n-1, n)) = \frac{(n-2)(n-3)}{2} - 2$ . Then  $A(i, n-1, n) \in \Gamma(n-3, n-4)$  and

$$f(A(i, n-1, n)) \leq \frac{(n-3)(n-4)}{2} \quad \text{for all } 1 \leq i \leq n-2. \quad (3.26)$$

Next we prove the following claim.

**Claim 2.** *Let  $i \in \{1, 2, \dots, n-2\}$ . Then*

$$f(A(i, n-1, n)) \leq \frac{(n-3)(n-4)}{2} - 1. \quad (3.27)$$

*Moreover, there exists some  $i \in \{1, 2, \dots, n-2\}$  such that equality in (3.27) holds.*

Suppose equality in (3.26) holds for some  $i$ , say,  $i = n-2$ . By Theorem 3,  $A(n-2, n-1, n)$  is permutation similar to  $T_{n-3}$ . Without loss of generality, we assume

$$A = \begin{bmatrix} T_{n-3} & x_1 & x_2 & x_3 \\ y_1^T & a_{n-2, n-2} & a_{n-2, n-1} & a_{n-2, n} \\ y_2^T & a_{n-1, n-2} & a_{n-1, n-1} & a_{n-1, n} \\ y_3^T & a_{n, n-2} & a_{n, n-1} & a_{n, n} \end{bmatrix},$$

where  $x_i, y_i \in \mathbb{R}^{n-3}$ , for  $i = 1, 2, 3$ . Since  $\delta_{n-2} \geq n-2$  and

$$f(x_1) + f(y_1) + a_{n-2, n-2} = f(A(n-1, n)) - f(A(n-2, n-1, n)) = n-5,$$

we have

$$\sum_{i=n-1, n} (a_{n-2, i} + a_{i, n-2}) = \delta_{n-2} - [f(x_1) + f(y_1) + a_{n-2, n-2}] \geq 3.$$

Then either  $a_{n-2, n-1} + a_{n-1, n-2} = 2$  or  $a_{n-2, n} + a_{n, n-2} = 2$ . Without loss of generality, we assume  $a_{n-1, n-2} = a_{n-2, n-1} = 1$ . By Lemma 1 (ii) of [8], we obtain  $a_{n-1, n-1} = a_{n-2, n-2} = 0$  and

$$f(x_1) + f(y_1) = n-5 \geq 4.$$

Then we have  $f(x_1) \geq 3$  or  $f(y_1) \geq 3$ , or  $f(x_1) = f(y_1) = 2$ . Applying Lemma 11 to  $A(n)$ , we get  $D \notin Ex(n, \mathcal{F}_{n-4})$ , a contradiction.

Therefore, (3.26) is a strict inequality and we have (3.27). Moreover, applying Lemma 4 to  $A(n-1, n)$  we get the second part of Claim 2.

Without loss of generality we assume

$$f(A(n-2, n-1, n)) = \frac{(n-3)(n-4)}{2} - 1.$$

For any  $i \in \{1, 2, \dots, n-3\}$ , since  $A(i, n-2, n-1, n) \in \Gamma(n-4, n-4)$ , by Theorem 3 we have

$$f(A(i, n-2, n-1, n)) \leq \frac{(n-4)(n-5)}{2}. \quad (3.28)$$

Applying Lemma 4 to  $A(n-2, n-1, n)$ , there is some  $i$ , say,  $i = n-3$  such that equality in (3.28) holds. It follows that  $A(n-3, n-2, n-1, n)$  is permutation similar to  $T_{n-4}$  and we may assume

$$A = (a_{ij}) = \begin{bmatrix} T_{n-4} & x_{n-3} & x_{n-2} & x_{n-1} & x_n \\ y_{n-3}^T & a_{n-3, n-3} & a_{n-3, n-2} & a_{n-3, n-1} & a_{n-3, n} \\ y_{n-2}^T & a_{n-2, n-3} & a_{n-2, n-2} & a_{n-2, n-1} & a_{n-2, n} \\ y_{n-1}^T & a_{n-1, n-3} & a_{n-1, n-2} & a_{n-1, n-1} & a_{n-1, n} \\ y_n^T & a_{n, n-3} & a_{n, n-2} & a_{n, n-1} & a_{n, n} \end{bmatrix}$$

where  $x_i, y_i \in \mathbb{R}^{n-4}$  for  $i = n, n-1, n-2, n-3$ .

Since

$$f(x_{n-3}) + f(y_{n-3}) + a_{n-3,n-3} = f(A(n-2, n-1, n)) - f(A(n-3, n-2, n-1, n)) = n-5,$$

applying Lemma 9 to  $A(n-2, n-1, n)$  we have  $a_{n-3,n-3} = 0$  and

$$f(x_{n-3}) + f(y_{n-3}) = n-5 \geq 4. \quad (3.29)$$

We assert

$$a_{n-3,n-2}a_{n-2,n-3} = 0. \quad (3.30)$$

Otherwise  $a_{n-3,n-2} = a_{n-2,n-3} = 1$ . Applying Lemma 11 to  $A(n-1, n)$  we can deduce  $A \notin \Gamma(n, n-4)$ , a contradiction.

Similarly, we have

$$a_{n-3,i}a_{i,n-3} = 0 \quad \text{for } i = n-1, n.$$

It follows that

$$\sum_{i=n-2}^n (a_{n-3,i} + a_{i,n-3}) \leq 3.$$

On the other hand,

$$\sum_{i=n-2}^n (a_{n-3,i} + a_{i,n-3}) = \delta_{n-3} - f(x_{n-3}) - f(y_{n-3}) \geq n-2 - (n-5) = 3.$$

Hence, we have  $\sum_{i=n-2}^n (a_{n-3,i} + a_{i,n-3}) = 3$  and

$$a_{n-3,i} + a_{i,n-3} = 1 \quad \text{for } i = n-2, n-1, n.$$

Applying Lemma 9 to  $A(n-3, n-1, n)$  we obtain  $a_{n-2,n-2} = 0$  and

$$\begin{aligned} & f(x_{n-2}) + f(y_{n-2}) \\ &= f(A(n-1, n)) - f(A(n-2, n-1, n)) - a_{n-2,n-2} - a_{n-3,n-2} - a_{n-2,n-3} \\ &= n-5. \end{aligned}$$

Repeating the above arguments, we get

$$a_{n-2,i} + a_{i,n-2} = 1 \quad \text{for } i = n-1, n$$

and

$$a_{n-1,n-1} = a_{nn} = 0, \quad a_{n-1,n} + a_{n,n-1} = 1.$$

Moreover, we have

$$f(x_{n-i}) + f(y_{n-i}) = n-5 \quad \text{for } i = 0, 1, 2, 3. \quad (3.31)$$

Now we verify

**Claim 3.**  $B \equiv A[n-3, n-2, n-1, n]$  is permutation similar to  $T_4$ .

It is well known that the adjacency matrix of an acyclic digraph is permutation similar to a strictly upper triangular matrix. Suppose Claim 3 does not hold. Then the digraph  $D(B)$  has at least one cycle. Note that  $a_{ii} = 0$  and  $a_{ij}a_{ji} = 0$  for  $i, j = n-3, \dots, n$ .  $D(B)$  has no loop or 2-cycle. If  $D(B)$  has a 4-cycle, then  $B$  is permutation similar to

$$B' = \begin{bmatrix} 0 & 1 & b_{13} & 0 \\ 0 & 0 & 1 & b_{24} \\ b_{31} & 0 & 0 & 1 \\ 1 & b_{42} & 0 & 0 \end{bmatrix}.$$

Now  $b_{24} = 1$  implies  $D(B)$  has a cycle  $1 \rightarrow 2 \rightarrow 4 \rightarrow 1$  of length 3;  $b_{42} = 1$  implies  $D(B)$  has a cycle  $2 \rightarrow 3 \rightarrow 4 \rightarrow 2$  of length 3. Therefore,  $D$  always has a 3-cycle with vertices from  $\{n-3, n-2, n-1, n\}$ . Without loss of generality, we assume the 3-cycle is  $n-3 \rightarrow n-2 \rightarrow n-1 \rightarrow n-3$ .

Applying Lemma 11 to  $A(n)$ , we get

$$f(x_i) \leq 2 \text{ and } f(y_i) \leq 2 \text{ for } i = n-3, n-2, n-1.$$

By (3.31) we have  $n = 9$  and

$$f(x_i) = f(y_i) = 2 \text{ for } i = n-3, n-2, n-1.$$

Suppose  $a_{j_1,6} = a_{j_2,6} = a_{8,j_3} = a_{8,j_4} = 1$  with  $1 \leq j_1 < j_2 \leq n-4 = 5$  and  $1 \leq j_3 < j_4 \leq 5$ . Then  $D$  has two distinct walks from  $j_1$  to  $j_4$  of length  $n-4$ :

$$\begin{cases} j_1 \rightarrow 6 \rightarrow 7 \rightarrow 8 \rightarrow j_3 \rightarrow j_4, \\ j_1 \rightarrow j_2 \rightarrow 6 \rightarrow 7 \rightarrow 8 \rightarrow j_4, \end{cases}$$

a contradiction. Therefore,  $D(B)$  is acyclic and Claim 3 holds.

Without loss of generality, we assume

$$A = \begin{bmatrix} T_{n-4} & x_{n-3} & x_{n-2} & x_{n-1} & x_n \\ y_{n-3}^T & 0 & 1 & 1 & 1 \\ y_{n-2}^T & 0 & 0 & 1 & 1 \\ y_{n-1}^T & 0 & 0 & 0 & 1 \\ y_n^T & 0 & 0 & 0 & 0 \end{bmatrix}.$$

For  $i = n, n-1, n-2, n-3$ , let  $a_{s_i,i}$  be the last nonzero component in  $x_i$  and  $a_{i,t_i}$  be the first nonzero component in  $y_i$ , where  $s_i \equiv 0$  if  $x_i = 0$  and  $t_i \equiv n-3$  if  $y_i = 0$ . Applying

Lemma 9 to  $A(n-2, n-1, n)$ ,  $A(n-3, n-1, n)$ ,  $A(n-3, n-2, n)$  and  $A(n-3, n-2, n-1)$ , we have

$$x_i = (a_i^T, 0)^T, \quad y_i = (0, b_i^T)^T \quad \text{for } i = n-3, n-2, n-1, n, \quad (3.32)$$

where  $a_i \in \mathbb{R}^{s_i}$ ,  $b_i \in \mathbb{R}^{n-s_i-4}$ . Moreover, by (3.31) we have

$$s_i < t_i \leq s_i + 2 \quad \text{for } i = n, n-1, n-2, n-3. \quad (3.33)$$

Next, we verify the following claim.

**Claim 4.** *If  $n-3 \leq i < j \leq n$ , then*

$$t_j > s_i + 1. \quad (3.34)$$

We assert

$$a_{ij} = 0 \quad \text{for } n-5 \leq i \leq n-4, n-3 \leq j \leq i+3. \quad (3.35)$$

Otherwise,  $D$  has the following two distinct walks of length  $n-4$  from 1 to  $j+1$  or  $j+2$ :

$$\begin{cases} 1 \rightarrow 2 \rightarrow 4 \rightarrow \cdots \rightarrow i \rightarrow j \rightarrow j+1 (\rightarrow j+2), \\ 1 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \rightarrow i \rightarrow j \rightarrow j+1 (\rightarrow j+2). \end{cases}$$

Similarly, we have  $a_{i1} = 0$  for  $i = n-2, n-1, n$ . Otherwise,  $D$  has the following two distinct walks of length  $n-4$  from  $i-1$  to  $n-4$ :

$$\begin{cases} i-1 \rightarrow i \rightarrow 1 \rightarrow 2 \rightarrow 4 \rightarrow \cdots \rightarrow n-4, \\ i-1 \rightarrow i \rightarrow 1 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \rightarrow n-4. \end{cases}$$

Given any  $n-3 \leq i < j \leq n$ , we have

$$t_j \geq 2 \quad \text{for } n-2 \leq j \leq n$$

and

$$s_i \leq n-5 \quad \text{for } n-3 \leq i \leq n-1.$$

If  $s_i = 0$ , then  $t_j > s_i + 1$  and (3.34) holds. For  $s_i \geq 1$ , if (3.34) does not hold, we can distinguish the following cases to find two distinct walks of length  $n-4$  between the same endpoints to deduce contradictions.

*Subcase 1.*  $t_j = s_i + 1$ . If  $s_i = 1$ , then  $t_j = 2$  and  $D$  has

$$\begin{cases} 1 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 4 \rightarrow 5 \rightarrow \cdots \rightarrow n-4, \\ 1 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 3 \rightarrow 5 \rightarrow \cdots \rightarrow n-4. \end{cases}$$

If  $s_i = 2$  and  $a_{1i} = 0$ , then by (3.31) and (3.32),  $t_j = 3$ ,  $t_i = s_i + 1 = 3$  and  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4, \\ 1 \rightarrow 2 \rightarrow i \rightarrow t_i \rightarrow 4 \rightarrow 5 \rightarrow \cdots \rightarrow n-4. \end{cases}$$

If  $s_i = 2$  and  $a_{1i} = 1$ , then  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4, \\ 1 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 4 \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4. \end{cases}$$

If  $s_i = 3$  and  $a_{2i} = 0$ , then  $t_i = s_i + 1 = 4$  and  $D$  has

$$\begin{cases} 1 \rightarrow 3 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4, \\ 1 \rightarrow 2 \rightarrow 3 \rightarrow i \rightarrow t_i \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4. \end{cases}$$

If  $s_i = 3$  and  $a_{2i} = 1$ , then  $D$  has

$$\begin{cases} 1 \rightarrow 3 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4, \\ 1 \rightarrow 2 \rightarrow i \rightarrow j \rightarrow t_j \rightarrow 5 \rightarrow 6 \rightarrow \cdots \rightarrow n-4. \end{cases}$$

If  $4 \leq s_i \leq n-5$ , then  $D$  has

$$\begin{cases} 1 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow j \rightarrow t_j \rightarrow t_j + 1 \rightarrow \cdots \rightarrow n-4, \\ 1 \rightarrow 2 \rightarrow 4 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow j \rightarrow t_j \rightarrow t_j + 1 \rightarrow \cdots \rightarrow n-4, \end{cases}$$

where the walk  $t_j \rightarrow t_j + 1 \rightarrow \cdots \rightarrow n-4$  does not appear when  $s_i = n-5$ .

*Subcase 2.*  $t_j < s_i + 1$ . Since  $t_j \geq 2$  for  $j = n-2, n-1, n$ , we have  $s_i \geq 2$ . If  $s_i = 2$  or 3,  $D$  has the same walks as in the previous subcase. If  $4 \leq s_i \leq n-5$ , the walks

$$\begin{cases} 1 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow j \rightarrow t_j \rightarrow s_i + 1 \rightarrow \cdots \rightarrow n-4 \\ 1 \rightarrow 2 \rightarrow 4 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow j \rightarrow t_j \rightarrow s_i + 1 \rightarrow \cdots \rightarrow n-4 \end{cases}$$

contain two walks of length  $n-4$  with the same endpoints.

Thus we obtain Claim 4.

Now we show

**Claim 5.**  $s_i \neq s_j$  for  $n-3 \leq i < j \leq n$ .

Suppose  $s_k = s_l$  for some  $n-3 \leq k < l \leq n$ . Then by the definition of  $s_i$  we have

$$a_{s_k+1,k} = a_{s_k+1,l} = 0. \quad (3.36)$$

From (3.32) we have

$$a_{s_k+1,j} + a_{j,s_k+1} \leq 1 \quad \text{for } j = n-3, n-2, n-1, n. \quad (3.37)$$

By (3.21),

$$\delta_{s_k+1} = n - 5 + \sum_{j=n-3}^n (a_{s_k+1,j} + a_{j,s_k+1}) \geq n - 2.$$

Combining this with (3.36) and (3.37) we have

$$a_{k,s_k+1} + a_{l,s_k+1} \geq 1.$$

By (3.33) and (3.34), we have  $t_l = s_l + 2$ . Hence,

$$a_{l,s_k+1} = 0 \quad \text{and} \quad a_{k,s_k+1} = 1.$$

It follows that

$$t_k = s_k + 1. \tag{3.38}$$

If  $s_k = 0$ , then  $D$  has two distinct walks of length  $n - 4$  from  $k$  to  $n - 4$ :

$$\begin{cases} k \rightarrow 1 \rightarrow 2 \rightarrow \cdots \rightarrow n - 4, \\ k \rightarrow l \rightarrow 2 \rightarrow \cdots \rightarrow n - 4, \end{cases}$$

a contradiction. If  $1 \leq s_k \leq n - 6$ , then  $D$  has two distinct walks of length  $n - 4$  from 1 to  $n - 4$ :

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_k \rightarrow k \rightarrow l \rightarrow t_l \rightarrow t_l + 1 \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_k \rightarrow k \rightarrow t_k \rightarrow t_k + 1 \rightarrow \cdots \rightarrow n - 4, \end{cases}$$

a contradiction. Hence we have  $s_k \geq n - 5$ .

On the other hand, by (3.35) we have

$$s_{n-3} \leq n - 6, s_{n-2} \leq n - 6 \text{ and } s_{n-1} \leq n - 5.$$

It follows that

$$s_{n-3} \neq s_{n-2}, \quad k = n - 1, \quad l = n \quad \text{and} \quad s_k = n - 5.$$

Moreover, there exists  $s_m \geq 1$  with  $m \in \{n - 3, n - 2\}$ . Now we can distinguish the following cases to find distinct walks of length  $n - 4$  with the same endpoints in  $D$  to deduce contradictions.

If  $t_m = s_m + 1$ , then by (3.38)  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_m \rightarrow m \rightarrow s_m + 1 \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_k \rightarrow k \rightarrow n - 4. \end{cases}$$

If  $s_m + 2 = t_m \leq n - 5$ , then  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_m \rightarrow m \rightarrow t_m \rightarrow \cdots \rightarrow s_k \rightarrow k \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_k \rightarrow k \rightarrow n - 4. \end{cases}$$



If  $s_m + 2 = t_m = n - 4$ , then  $s_m = n - 6$  and  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_m \rightarrow m \rightarrow k \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_k \rightarrow k \rightarrow n - 4. \end{cases}$$

Hence we get Claim 5.

Combining Claim 4 and Claim 5 we obtain

$$s_j > s_i \text{ for } n - 3 \leq i < j \leq n.$$

Otherwise,  $s_j < s_i$  leads to  $t_j \leq s_j + 2 < s_i + 2$ , which contradicts Claim 4. Therefore, we have

$$0 \leq s_{n-3} < s_{n-2} < s_{n-1} < s_n \leq n - 4. \quad (3.39)$$

Finally, we verify

**Claim 6.**  $t_i = s_i + 2$  for  $i \in \{n - 3, n - 2, n - 1, n\}$ .

Suppose  $t_n = s_n + 1$ . By (3.39) and (3.33) we have  $1 \leq s_{n-2} \leq n - 6$  and  $s_n \geq t_{n-2}$ . We can distinguish the following cases to find two distinct walks of length  $n - 4$  from 1 to  $n - 4$  or  $n$  in  $D$ , which contradicts  $D \in Ex(n, \mathcal{F}_{n-4})$ . If  $t_{n-2} = s_{n-2} + 2$ , then  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_n \rightarrow n \rightarrow s_n + 1 \rightarrow s_n + 2 \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_{n-2} \rightarrow n - 2 \rightarrow s_{n-2} + 2 \rightarrow \cdots \rightarrow s_n \rightarrow n \rightarrow s_n + 1 \rightarrow \cdots \rightarrow n - 4, \end{cases}$$

where the walk  $n \rightarrow s_n + 1 \rightarrow \cdots \rightarrow n - 4$  does not appear when  $s_n = n - 4$ . If  $t_{n-2} = s_{n-2} + 1$  and  $s_n \leq n - 5$ , then  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_n \rightarrow n \rightarrow s_n + 1 \rightarrow s_n + 2 \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_{n-2} \rightarrow n - 2 \rightarrow s_{n-2} + 1 \rightarrow s_{n-2} + 2 \rightarrow \cdots \rightarrow n - 4. \end{cases}$$

If  $t_{n-2} = s_{n-2} + 1$  and  $s_n = n - 4$ , then  $a_{n-4,n} = 1$  and  $D$  has

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow n - 5 \rightarrow n - 4 \rightarrow n, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_{n-2} \rightarrow n - 2 \rightarrow t_{n-2} \rightarrow t_{n-2} + 2 \rightarrow \cdots \rightarrow n - 4 \rightarrow n, \text{ if } s_{n-2} \leq n - 7, \\ 1 \rightarrow 3 \rightarrow \cdots \rightarrow s_{n-2} \rightarrow n - 2 \rightarrow t_{n-2} \rightarrow t_{n-2} + 1 \rightarrow \cdots \rightarrow n - 4 \rightarrow n, \text{ if } s_{n-2} = n - 6. \end{cases}$$

Hence,  $t_n = s_n + 2$  and  $s_n \leq n - 5$ .

Next suppose  $t_i = s_i + 1$  for  $i \in \{n - 2, n - 1\}$  and  $j \in \{n - 2, n - 1\} \setminus \{i\}$ . Then  $s_i, s_j > 0$ . If  $t_j = s_j + 1$ , then  $D$  has the following two distinct walks of length  $n - 4$  from 1 to  $n - 4$ :

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow s_i + 1 \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_j \rightarrow j \rightarrow s_j + 1 \rightarrow \cdots \rightarrow n - 4, \end{cases}$$

a contradiction. If  $t_j = s_j + 2$ , then  $D$  has the following two distinct walks of length  $n - 4$  from 1 to  $n - 4$ :

$$\begin{cases} 1 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow s_i + 1 \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow s_i + 1 \rightarrow \cdots \rightarrow s_j \rightarrow j \rightarrow s_j + 2 \rightarrow \cdots \rightarrow n - 4, & \text{if } i < j, \\ 1 \rightarrow \cdots \rightarrow s_j \rightarrow j \rightarrow s_j + 2 \rightarrow \cdots \rightarrow s_i \rightarrow i \rightarrow s_i + 1 \rightarrow \cdots \rightarrow n - 4, & \text{if } i > j \text{ and } s_i \geq s_j + 2 \\ 1 \rightarrow \cdots \rightarrow s_j \rightarrow j \rightarrow i \rightarrow s_i + 1 \rightarrow \cdots \rightarrow n - 4, & \text{if } i > j \text{ and } s_i = s_j + 1, \end{cases}$$

a contradiction. Hence, we get

$$t_{n-2} = s_{n-2} + 2, \quad t_{n-1} = s_{n-1} + 2.$$

Now we conclude  $t_{n-3} = s_{n-3} + 2$ . Otherwise  $D$  has the following two distinct walks of length  $n - 4$  from 1 or  $n - 3$  to  $n - 4$ :

$$\begin{cases} 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_{n-3} \rightarrow n - 3 \rightarrow t_{n-3} \rightarrow \cdots \rightarrow n - 4, \\ 1 \rightarrow 2 \rightarrow \cdots \rightarrow s_{n-3} \rightarrow n - 3 \rightarrow t_{n-3} \rightarrow \cdots \rightarrow s_{n-1} \rightarrow n - 1 \rightarrow s_{n-1} + 2 \rightarrow \cdots \rightarrow n - 4, \end{cases}$$

where the walk  $1 \rightarrow 2 \rightarrow \cdots \rightarrow s_{n-3} \rightarrow n - 3$  does not appear when  $s_{n-3} = 0$ . Thus we get Claim 6.

Finally, combining (3.31) and Claim 6 we have  $A = F_4(n)$ . This completes the proof.  $\square$

From the proof of Theorem 12, we have the following corollary.

**Corollary 13.** *Let  $k \geq 5$  be an integer,  $n = k + 4$  and*

$$A = (a_{ij}) = \begin{bmatrix} T_k & B \\ C & E \end{bmatrix} \in \Gamma(n, k).$$

*If*

$$\begin{aligned} f(A) &= \frac{n(n-1)}{2} - 4, & f(A(n)) &= \frac{(n-1)(n-2)}{2} - 3, \\ f(A(n-1, n)) &= \frac{(n-2)(n-3)}{2} - 2, & f(A(n-2, n-1, n)) &= \frac{(n-3)(n-4)}{2} - 1, \end{aligned}$$

*then  $A$  is permutation similar to  $F_4(n)$  by permuting its last 4 rows and columns.*

## 4 Proof of Theorem 2

In this section we give the proof of Theorem 2. We will use induction on  $n$ . First we need the following lemma to show that Theorem 2 holds for  $k = 5$ .

**Lemma 14.** *Let  $n \geq 10$  be an integer. Then*

$$ex(n, \mathcal{F}_{n-5}) = \frac{n(n-1)}{2} - 5. \quad (4.1)$$

*Moreover, a digraph  $D$  is in  $Ex(n, \mathcal{F}_{n-5})$  if and only if  $D$  is a  $(1, n-5, 5)$ -completely transitive tournament.*

*Proof.* Let  $D$  be any  $\mathcal{F}_{n-5}$ -free digraph of order  $n$ . Denote by  $A \equiv A_D$ . Given any  $i \in \{1, 2, \dots, n\}$ , since  $A(i) \in \Gamma(n-1, n-5)$ , by Theorem 10 we have

$$f(A(i)) \leq \frac{(n-1)(n-2)}{2} - 4. \quad (4.2)$$

Applying Lemma 4 to  $A$ , we have

$$f(A) \leq \frac{n(n-1)}{2} - 5.$$

Hence,

$$ex(n, \mathcal{F}_{n-5}) \leq \frac{n(n-1)}{2} - 5.$$

Let  $D$  be any  $(1, n-5, 5)$ -completely transitive tournament. Then  $A_D$  is a principal submatrix of  $A' = J_2 \otimes T_{n-5}$ . Since  $A'(\alpha) \in \Gamma(n, n-5)$ , the digraph  $D(A')$ , and hence  $D$  is  $\mathcal{F}_{n-5}$ -free. It is clear that  $D$  has size  $\frac{n(n-1)}{2} - 5$ . Thus we get (4.1) and the sufficiency of the second part.

Let  $D \in Ex(n, \mathcal{F}_{n-5})$  and  $A \equiv A_D$ . Again, denote by  $\delta_i$  the number of nonzero entries lying in the  $i$ -th row and the  $i$ -th column of  $A$ . Then by (4.2),

$$\delta_i = f(A) - f(A(i)) \geq n - 2 \quad \text{for all } 1 \leq i \leq n. \quad (4.3)$$

Applying Lemma 4 we get

$$f(A(i_0)) \geq \frac{(n-1)(n-2)}{2} - 4$$

for some  $i_0 \in \{1, 2, \dots, n\}$ . Without loss of generality, we assume  $i_0 = n$ . By Theorem 12,  $A(n)$  is permutation similar to  $F_t(n-1)$  with  $t \in \{1, 2, 3, 4\}$ . Now we distinguish four cases.

*Case 1.*  $A(n)$  is permutation similar to  $F_1(n-1)$ . Without loss of generality, we assume

$$A = \begin{bmatrix} 0 & J_{3,n-6} & J_{3,2} & x_1 \\ 0 & T_{n-6} & J_{n-6,2} & x_2 \\ 0 & 0 & 0 & x_3 \\ y_1^T & y_2^T & y_3^T & \alpha \end{bmatrix},$$

where  $x_1, y_1 \in \mathbb{R}^3$ ,  $x_2, y_2 \in \mathbb{R}^{n-6}$ ,  $x_3, y_3 \in \mathbb{R}^2$ .

Since

$$\delta_n = \sum_{i=1}^3 [f(x_i) + f(y_i)] + \alpha = f(A) - f(A(n)) = n - 2,$$

applying Lemma 5 to  $A$  we have

$$y_1 = 0 \text{ and } x_3 = 0.$$

Then  $\delta_1 \leq n - 3$ , which contradicts (4.3).

*Case 2.*  $A(n)$  is permutation similar to  $F_2(n - 1)$ . Applying the same arguments as in Case 1 we get  $\delta_{n-2} \leq n - 3$ , a contradiction.

*Case 3.*  $A(n)$  is permutation similar to  $F_3(n - 1)$ . Without loss of generality, we assume

$$A = \begin{bmatrix} 0 & J_{2,n-6} & J_{2,2} & J_{2,1} & x_1 \\ 0 & T_{n-6} & J_{n-6,2} & U_m & x_2 \\ 0 & 0 & 0 & 0 & x_3 \\ 0 & U'_m & J_{1,2} & 0 & a_{n-1,n} \\ y_1^T & y_2^T & y_3^T & a_{n,n-1} & a_{nn} \end{bmatrix}$$

where  $x_1, x_3, y_1, y_3 \in \mathbb{R}^2$ ,  $x_2, y_2 \in \mathbb{R}^{n-6}$ ,  $U_m = (J_{1,m}, 0)^T$ ,  $U'_m = (0, J_{1,n-m-8})$ ,  $0 \leq m \leq n - 8$ . By (4.3),

$$\delta_{n-1} = n - 4 + a_{n-1,n} + a_{n,n-1} \geq n - 2$$

implies  $a_{n-1,n} = a_{n,n-1} = 1$ . Applying Lemma 5 to  $A(n - 1)$  we get  $x_3 = 0$  and  $y_1 = 0$ . Hence,  $\delta_1 \geq n - 2$  and  $\delta_2 \geq n - 2$  force  $x_1 = J_{2,1}$ . Then  $D$  has the following two distinct walks of length  $n - 5$  from 1 to  $n - 1$  or  $n$ :

$$\begin{cases} 1 \rightarrow 2 \rightarrow n - 1 \rightarrow n \rightarrow n - 1 \rightarrow \cdots \rightarrow n - 1 (\rightarrow n), \\ 1 \rightarrow n \rightarrow n - 1 \rightarrow n \rightarrow n - 1 \rightarrow \cdots \rightarrow n - 1 (\rightarrow n), \end{cases}$$

a contradiction.

*Case 4.*  $A(n)$  is permutation similar to  $F_4(n - 1)$ . Without loss of generality we assume

$$A = (a_{ij}) = \begin{bmatrix} T_{n-5} & w_4 & w_3 & w_2 & w_1 & x \\ u_4 & 0 & 1 & 1 & 1 & a_{n-4,n} \\ u_3 & 0 & 0 & 1 & 1 & a_{n-3,n} \\ u_2 & 0 & 0 & 0 & 1 & a_{n-2,n} \\ u_1 & 0 & 0 & 0 & 0 & a_{n-1,n} \\ y^T & a_{n,n-4} & a_{n,n-3} & a_{n,n-2} & a_{n,n-1} & a_{n,n} \end{bmatrix} \equiv \begin{bmatrix} T_{n-5} & B \\ C & E \end{bmatrix},$$

where  $x, y \in \mathbb{R}^{n-5}$ ,

$$w_i = (J_{1,q_i}, 0)^T, \quad u_i = (0, J_{1,n-q_i-6}) \quad \text{for } i \in \{1, 2, 3, 4\}$$

with  $0 \leq q_4 < q_3 < q_2 < q_1 \leq n - 6$ .

We claim

$$a_{n-i,n}a_{n,n-i} = 0 \quad \text{for } i = 1, 2, 3, 4. \quad (4.4)$$

Otherwise suppose  $a_{n-i,n} = a_{n,n-i} = 1$  for some  $i \in \{1, 2, 3, 4\}$ . Set

$$\alpha = \{1, 2, \dots, n-5, n-i, n\}.$$

Applying Lemma 11 to  $A[\alpha]$  we get  $A \notin \Gamma(n, n-5)$ , a contradiction. Thus we obtain (4.4).

On the other hand, by (4.3) we have

$$a_{n,n-i} + a_{n-i,n} = \delta_{n-i} - f(w_i) - f(u_i) - 3 \geq 1 \quad \text{for } i \in \{1, 2, 3, 4\}.$$

Hence, we have  $a_{n,n-i} + a_{n-i,n} = 1$ , and

$$f(A(n-i)) = f(A) - \delta_{n-i} = \frac{(n-1)(n-2)}{2} - 4 \quad \text{for } i = 1, 2, 3, 4.$$

Given  $i \in \{1, 2, 3, 4, 5\}$ , applying Corollary 13 to  $A(n-i)$  we know each  $4 \times 4$  principal submatrix of  $E$  is permutation similar to  $T_4$ . Let  $w_5 = x$  and  $u_5 = y^T$ . By Lemma 9 of [8],  $E$  is permutation similar to  $T_5$  and  $A$  is permutation similar to

$$H = \begin{bmatrix} T_{n-5} & w_{\sigma_1} & w_{\sigma_2} & w_{\sigma_3} & w_{\sigma_4} & w_{\sigma_5} \\ u_{\sigma_1} & 0 & 1 & 1 & 1 & 1 \\ u_{\sigma_2} & 0 & 0 & 1 & 1 & 1 \\ u_{\sigma_3} & 0 & 0 & 0 & 1 & 1 \\ u_{\sigma_4} & 0 & 0 & 0 & 0 & 1 \\ u_{\sigma_5} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

with  $\sigma$  a permutation of  $\{1, 2, 3, 4, 5\}$ . Applying Corollary 13 to each  $A(n-i)$  again we get

$$w_{\sigma_i} = (J_{1,k_i}, 0)^T, \quad u_{\sigma_i} = (0, J_{1,n-k_i-6}) \quad \text{for } i = 1, 2, 3, 4, 5$$

with  $0 \leq k_1 < k_2 < k_3 < k_4 < k_5 \leq n - 6$ .

Denote  $G = J_2 \otimes T_{n-5}$  and

$$\beta = \{n-4, n-5, \dots, 2(n-5)\} \setminus \{n-4+k_1, n-4+k_2, n-4+k_3, n-4+k_4, n-4+k_5\}.$$

Then  $H = G(\beta)$  and  $D$  is a  $(1, n-5, 5)$ -completely transitive tournament.  $\square$

Now we are ready to present the proof of Theorem 2.

**Proof of Theorem 2.** We use induction on  $n$ . By Theorem 10 and Lemma 14 we know the results hold for  $n = k+4$  and  $n = k+5$ . Assume the results hold for  $n = k+5, \dots, sk+t$ , where  $0 \leq t < k$  and  $s > 0$  are integers.

Now suppose  $n = sk + t + 1$ . Let  $u, v$  be integers such that  $v < k$  and  $n = uk + v$ . Then  $u = s, v = t + 1$  when  $t < k - 1$ , and  $u = s + 1, v = 0$  when  $t = k - 1$ .

Given any  $\mathcal{F}_k$ -free digraph  $D$  of order  $n$ , denote by  $A \equiv A_D$  its adjacency matrix. For any  $i \in \{1, 2, \dots, n\}$ , since the digraph of  $A(i)$  is an  $\mathcal{F}_k$ -free digraph of order  $n - 1$ , by the induction hypothesis we have

$$\begin{aligned} f(A(i)) &\leq ex(n - 1, \mathcal{F}_k) \\ &= \binom{n - 1}{2} - \binom{s}{2}k - st \\ &= \frac{(n - 1)(n - 2)}{2} - \frac{(s - 1)(n - 1)}{2} - \frac{(s + 1)t}{2}. \end{aligned} \quad (4.5)$$

Applying Lemma 4 we have

$$\begin{aligned} f(A) &\leq \frac{n(n - 1)}{2} - \frac{(s - 1)(n - 1)}{2} - \frac{(s + 1)t}{2} - s \\ &= \frac{n(n - 1)}{2} - \frac{(s - 1)n}{2} - \frac{(s + 1)(t + 1)}{2} \\ &= \frac{n(n - 1)}{2} - \frac{(u - 1)n}{2} - \frac{(u + 1)v}{2}. \end{aligned}$$

Hence,

$$ex(n, \mathcal{F}_k) \leq \frac{n(n - 1)}{2} - \frac{(u - 1)n}{2} - \frac{(u + 1)v}{2}.$$

On the other hand, if  $D$  is a  $(u, k, v)$ -completely transitive tournament, then there exist  $k - t$  numbers  $j_1, j_2, \dots, j_{k-t} \in \{uk + 1, uk + 2, \dots, (u + 1)k\}$  such that

$$PAP^T = \Pi_{u+1,k}(j_1, j_2, \dots, j_{k-v})$$

for some permutation matrix  $P$ . Since  $(\Pi_{u+1,k})^k = 0$ , we have  $(A_D)^k = 0$ , and hence  $D$  is  $\mathcal{F}_k$ -free. Moreover, the size of  $D$  is

$$f(A) = \frac{n(n - 1)}{2} - \frac{(u - 1)n}{2} - \frac{(u + 1)v}{2}.$$

Hence,

$$ex(n, \mathcal{F}_k) = \frac{n(n - 1)}{2} - \frac{(u - 1)n}{2} - \frac{(u + 1)v}{2} = \binom{n}{2} - \binom{u}{2}k - uv \quad (4.6)$$

and any  $(u, k, v)$ -completely transitive tournament is in  $Ex(n, \mathcal{F}_k)$ .

Conversely, suppose  $D \in Ex(n, \mathcal{F}_k)$  and  $A \equiv A_D$ . Applying Lemma 4 to  $A$ , by (4.6) we know there is some  $i_0 \in \{1, 2, \dots, n\}$  such that equality in (4.5) holds. Without loss of generality, we assume  $i_0 = n$ . We distinguish two cases.

Case 1.  $t = 0$ . Then  $u = s \geq 2$  and  $v = 1$ . By the induction hypothesis we may assume

$$A = \begin{bmatrix} T_k & T_k & \cdots & T_k & x_1 \\ T_k & T_k & \cdots & T_k & x_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ T_k & T_k & \cdots & T_k & x_s \\ y_1^T & y_2^T & \cdots & y_s^T & a_{n,n} \end{bmatrix} \in M_{sk+1}\{0, 1\}, \quad (4.7)$$

where  $x_i, y_i \in \mathbb{R}^k$  for  $i = 1, 2, \dots, s$ .

Let  $a_{s_i, n}$  be the last nonzero component in  $x_i$ , and  $a_{n, t_i}$  be the first nonzero component in  $y_i$  for  $i = 1, \dots, s$ . Here we define  $s_i = (i-1)k$  when  $x_i = 0$ , and  $t_i = ik + 1$  when  $y_i = 0$ .

We claim

$$t_i \neq s_i + 1 \quad \text{for } 1 \leq i \leq s. \quad (4.8)$$

Note that we can change the role of each  $(x_i, y_i)$  by permutation similarity. To prove (4.8) it suffices to verify the case  $i = 1$ . Suppose  $t_1 = s_1 + 1$ . If  $s_1 \leq 2$ , then  $D$  has two distinct walks of length  $k$  from 1 or  $n$  to  $k$ :

$$\begin{cases} 1 \rightarrow \cdots \rightarrow s_1 \rightarrow n \rightarrow s_1 + 1 \rightarrow s_1 + 2 \rightarrow s_1 + 3 \rightarrow \cdots \rightarrow k, \\ 1 \rightarrow \cdots \rightarrow s_1 \rightarrow n \rightarrow s_1 + 1 \rightarrow k + s_1 + 2 \rightarrow s_1 + 3 \rightarrow \cdots \rightarrow k, \end{cases}$$

where the walk  $1 \rightarrow \cdots \rightarrow s_1$  does not appear when  $s_1 = 0$ . If  $3 \leq s_1 \leq k$ , then  $D$  has two distinct walks of length  $k$  from 1 to  $n$  or  $k$ :

$$\begin{cases} 1 \rightarrow 2 \rightarrow 3 \rightarrow \cdots \rightarrow s_1 \rightarrow n \rightarrow s_1 + 1 \rightarrow s_1 + 2 \rightarrow \cdots \rightarrow k, \\ 1 \rightarrow k + 2 \rightarrow 3 \rightarrow \cdots \rightarrow s_1 \rightarrow n \rightarrow s_1 + 1 \rightarrow s_1 + 2 \rightarrow \cdots \rightarrow k, \end{cases}$$

where the walk  $n \rightarrow s_1 + 1 \rightarrow s_1 + 2 \rightarrow \cdots \rightarrow k$  does not appear when  $s_1 = k$ . This contradicts  $D \in Ex(n, \mathcal{F}_k)$  and (4.8) follows.

Denote by

$$B_i = \begin{bmatrix} T_k & x_i \\ y_i^T & a_{nn} \end{bmatrix} \quad \text{for } 1 \leq i \leq s.$$

Given any  $i \in \{1, 2, \dots, s\}$ , since  $B_i$  is a principal submatrix of  $A$ , then  $B_i \in \Gamma(k+1, k)$ . By Theorem 3 we have  $f(B_i) \leq k(k+1)/2$  and

$$f(x_i) + f(y_i) + a_{nn} = f(B_i) - f(T_k) \leq k. \quad (4.9)$$

If equality in (4.9) holds, then applying Lemma 9 to  $B_i$  we get  $t_i = s_i + 1$ , which contradicts (4.8). Therefore, we have

$$f(x_i) + f(y_i) + a_{nn} \leq k - 1 \quad \text{for } 1 \leq i \leq s.$$

Since

$$\begin{aligned}
n - s - 1 = s(k - 1) &\geq \sum_{i=1}^s [f(x_i) + f(y_i) + a_{nn}] \\
&\geq \sum_{i=1}^s [f(x_i) + f(y_i)] + a_{nn} \\
&= f(A) - s^2 f(T_k) = n - s - 1
\end{aligned}$$

we get  $a_{nn} = 0$  and

$$f(x_i) + f(y_i) = k - 1 \quad \text{for } 1 \leq i \leq s.$$

By (4.8), applying Lemma 9 to each  $B_i$  again we have

$$t_i = s_i + 2 \quad \text{and} \quad x_i = (J_{1,q_i}, 0)^T, \quad y_i = (0, J_{1,k-q_i-1})^T \quad \text{with } q_i \in \{0, 1, \dots, k-1\}$$

for all  $1 \leq i \leq s$ . Now we assert

$$q_1 = q_2 = \dots = q_s = q \quad \text{for some } q \in \{0, 1, 2, \dots, k-1\}.$$

Otherwise, without loss of generality we assume  $q_1 < q_2$ . Then

$$s_1 = q_1, s_2 = k + q_2.$$

Denote by  $P$  the permutation matrix obtained by interchanging row  $q_1 + 1$  and row  $k + q_1 + 1$  of the  $n \times n$  identity matrix. Let  $A' = (a'_{ij}) = PAP^T$ . Then  $A' \in Ex(n, \mathcal{F}_k)$  has the same form (4.7) as  $A$ . Moreover, the last nonzero component in  $x_1$  is  $a'_{q_1+1,n} = a_{k+q_1+1,n}$ ; the first nonzero component in  $y_1$  is  $a'_{n,q_1+2} = a_{n,q_1+2}$ . If we define  $s'_i$  and  $t'_i$  for  $A'$  the same as  $s_i$  and  $t_i$  for  $A$ , then

$$s'_1 = q_1 + 1, \quad \text{and} \quad t'_1 = q_1 + 2.$$

On the other hand, using the same arguments as above we have  $t'_1 = s'_1 + 2$ , a contradiction.

Therefore, we have  $x_i = (J_{1,q}, 0)^T$ ,  $y_i = (0, J_{1,k-q-1})^T$  for  $i = 1, \dots, s$ , and  $A$  is permutation similar to  $\Pi_{s+1,k}(\beta)$  with  $\beta = \{sk + 1, sk + 2, \dots, sk + k\} \setminus \{q + 1\}$ . Hence,  $D$  is a  $(u, k, v)$ -completely transitive tournament.

Case 2.  $t \neq 0$ . By the induction hypothesis we may assume

$$A = \begin{bmatrix} T_k & T_k & \cdots & T_k & w_1 & w_2 & \cdots & w_t & x_1 \\ T_k & T_k & \cdots & T_k & w_1 & w_2 & \cdots & w_t & x_2 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\ T_k & T_k & \cdots & T_k & w_1 & w_2 & \cdots & w_t & x_s \\ u_1 & u_1 & \cdots & u_1 & 0 & 1 & \cdots & 1 & a_{sk+1,n} \\ u_2 & u_2 & \cdots & u_2 & 0 & 0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \ddots & 1 & a_{sk+t-1,n} \\ u_t & u_t & \cdots & u_t & 0 & 0 & \cdots & 0 & a_{sk+t,n} \\ y_1^T & y_2^T & \cdots & y_s^T & a_{n,sk+1} & a_{n,sk+2} & \cdots & a_{n,sk+t} & a_{nn} \end{bmatrix} \in M_{sk+t+1}\{0, 1\},$$



where  $x_i, y_i \in \mathbb{R}^k$  for  $i = 1, 2, \dots, s$ ,  $w_j = (J_{1,k_j}, 0)^T$ ,  $u_j = (0, J_{1,k-1-k_j})$ , and  $0 \leq k_1 < k_2 < \dots < k_t \leq k-1$ .

Let  $i \in \{1, 2, \dots, t\}$ . We claim

$$a_{sk+i,n} + a_{n,sk+i} = 1. \quad (4.10)$$

Since  $A(sk+i) \in \Gamma(n-1, k)$ , we have

$$\begin{aligned} a_{sk+i,n} + a_{n,sk+i} &= f(A) - f(A(sk+i)) - s[f(w_i) + f(u_i)] - (t-1) \\ &\geq f(A) - ex(n-1, \mathcal{F}_k) - s(k-1) - (t-1) = 1. \end{aligned} \quad (4.11)$$

If  $a_{sk+i,n} = a_{n,sk+i} = 1$ , setting

$$\alpha = \{1, 2, \dots, k, sk+i, n\}$$

and applying Lemma 11 to  $A[\alpha]$  we get  $A[\alpha] \notin \Gamma(k+2, k)$ , which contradicts  $A \in \Gamma(n, k)$ . Thus we get (4.10).

Combining (4.10) and (4.11) we get

$$f(A(sk+i)) = ex(n-1, \mathcal{F}_k).$$

By the induction hypothesis,  $A(sk+i)$  is permutation similar to a submatrix of  $\Pi_{s+1,k}$ . Therefore,  $a_{nn} = 0$  and

$$\sum_{i=1}^s [f(x_i) + f(y_i)] = f(A) - f(A(n)) - a_{nn} - \sum_{i=1}^t (a_{sk+i,n} + a_{n,sk+i}) = s(k-1).$$

Next we distinguish two subcases.

*Subcase 1.*  $s > 1$ . Let  $\alpha = \{sk+1, sk+2, \dots, sk+t\}$ . We consider  $A(\alpha)$ . Then

$$\begin{aligned} f(A(\alpha)) &= f(A) - s \sum_{i=1}^t [f(w_i) + f(u_i)] - t(t-1)/2 - \sum_{i=1}^t (a_{sk+i,n} + a_{n,sk+i}) - a_{nn} \\ &= \frac{n(n-1)}{2} - \frac{(s-1)n}{2} - \frac{(s+1)(t+1)}{2} - st(k-1) - t(t-1)/2 - t \\ &= \frac{(n-t)(n-t-1)}{2} - \frac{(s-1)(n-t)}{2} - \frac{s+1}{2} \\ &= ex(n-t, \mathcal{F}_k). \end{aligned}$$

Applying Case 1 to  $A(\alpha)$ , we have

$$x_j = (J_{1,q}, 0)^T \quad \text{and} \quad y_j^T = (0, J_{1,k-1-q})^T \quad \text{for all } j \in \{1, \dots, s\}$$

with  $0 \leq q \leq k-1$ .

We assert  $q \notin \{k_1, k_2, \dots, k_t\}$ . Otherwise suppose  $q = k_i$  for some  $i$ . Since

$$a_{q+1,n} = a_{n,q+1} = a_{q+1,sk+i} = a_{sk+i,q+1} = 0,$$

we have

$$\delta_{q+1} \leq s(k-1) + t - 1 = n - s - 2$$

and

$$f(A(q+1)) = f(A) - \delta_{q+1} > ex(n-1, \mathcal{F}_k),$$

which contradicts  $A(q+1) \in \Gamma(n-1, k)$ .

Next we show that

$$a_{sk+i,n} = 1 \text{ when } q > k_i \text{ for } i = 1, \dots, t.$$

Otherwise suppose  $q > k_i$  and  $a_{sk+i,n} = 0$ . Then by (4.10) we have  $a_{sk+i,q+1} = a_{n,sk+i} = 1$ . If  $q \leq 2$ , then  $D$  has two distinct walks of length  $k$  from 1 to  $k$ :

$$\begin{cases} 1 \rightarrow \dots \rightarrow q \rightarrow n \rightarrow sk+i \rightarrow q+1 \rightarrow q+2 \rightarrow q+3 \rightarrow \dots \rightarrow k-1 \rightarrow k, \\ 1 \rightarrow \dots \rightarrow q \rightarrow n \rightarrow sk+i \rightarrow q+1 \rightarrow k+q+2 \rightarrow q+3 \rightarrow \dots \rightarrow k, \end{cases}$$

a contradiction. If  $q \geq 3$ , then  $D$  has two distinct walks of length  $k$  from 1 to  $k$ :

$$\begin{cases} 1 \rightarrow 3 \rightarrow \dots \rightarrow q \rightarrow n \rightarrow sk+i \rightarrow q+1 \rightarrow \dots \rightarrow k-1 \rightarrow k, \\ 1 \rightarrow 2 \rightarrow \dots \rightarrow q-1 \rightarrow n \rightarrow sk+i \rightarrow q+1 \rightarrow \dots \rightarrow k-1 \rightarrow k, \end{cases}$$

a contradiction.

Using similar arguments as above, we can deduce  $a_{sk+i,n} = 0$  when  $q < k_i$ . Let

$$\beta = \{sk+1, sk+2, \dots, n\} \setminus \{sk+k_1+1, sk+k_2+1, \dots, sk+k_t+1, sk+q+1\}.$$

If  $q > k_t$ , then  $A = \Pi_{s+1,k}(\beta)$ . Otherwise let

$$P = \begin{cases} \begin{bmatrix} 0 & 1 \\ I_t & 0 \end{bmatrix}, & \text{if } q < k_1, \\ \begin{bmatrix} I_j & 0 & 0 \\ 0 & 0 & 1 \\ 0 & I_{t-j} & 0 \end{bmatrix}, & \text{if } k_j < q < k_j+1, \end{cases}$$

and  $Q = I_{sk} \oplus P$ . Then  $QAQ^T = \Pi_{s+1,k}(\beta)$ . Therefore,  $A$  is permutation similar to  $\Pi_{s+1,k}(\beta)$  and  $D$  is a  $(u, k, v)$ -completely transitive tournament.

*Subcase 2.*  $s = 1$ . Then  $t \geq 5$  and

$$A = (a_{ij}) = \begin{bmatrix} T_k & w_1 & w_2 & \dots & w_t & x \\ u_1 & 0 & 1 & \dots & 1 & a_{k+1,n} \\ u_2 & 0 & 0 & \ddots & \vdots & \vdots \\ \vdots & 0 & 0 & \ddots & 1 & \vdots \\ u_t & 0 & 0 & 0 & 0 & a_{k+t,n} \\ y^T & a_{n,k+1} & a_{n,k+2} & \dots & a_{n,k+t} & 0 \end{bmatrix} \in M_n\{0, 1\},$$

where  $x, y \in \mathbb{R}^{n-5}$ ,  $w_i = (J_{1,k_i}, 0)^T$ ,  $u_i = (0, J_{1,k-1-k_i})$ , and  $0 \leq k_1 < k_2 < \dots < k_t \leq k-1$ .

Choose any three distinct numbers  $p, q, r \in \{1, 2, \dots, t\}$ . Denote  $\alpha = \{1, 2, \dots, k, k+p, k+q, k+r, n\}$  and  $B = A[\alpha]$ . Then

$$f(B) = f(T_k) + 3(k-1) + 3 + f(x) + f(y) + 3 = (k+4)(k+3)/2 - 4 = ex(k+4, \mathcal{F}_k).$$

Applying Corollary 13 to  $B$ , we have

$$x = (J_{1,h}, 0)^T, \quad y = (0, J_{1,k-h-l})^T,$$

where  $0 \leq h \leq k-1$ . Moreover, we have  $h \notin \{k_p, k_q, k_r\}$  and

$$a_{k+i,n} = \begin{cases} 1, & \text{if } h > k_i, \\ 0, & \text{if } h < k_i, \end{cases} \quad (4.12)$$

for  $i = p, q, r$ .

Since  $p, q, r$  are arbitrarily chosen from  $\{1, 2, \dots, t\}$ , we have

$$h \notin \{k_1, k_2, \dots, k_t\}$$

and (4.12) holds for  $i = 1, 2, \dots, t$ . Using the same arguments as in the previous subcase, we can prove that  $D$  is a  $(u, k, v)$ -completely transitive tournament.

This completes the proof.  $\square$

## 5 Further discussion

In this section we discuss the unsolved cases for Problem 1. We focus our attention on strict digraphs. The second part of Theorem 2 may not be true for  $n = k+5$  when  $k = 4$ . For example, let  $D$  be the digraph with adjacency matrix

$$A = \begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}.$$

Then  $f(A) = 30$  and  $A^4 \in M_9\{0, 1\}$ . But  $A$  is not permutation similar to any principal submatrix of  $\Pi_{4,3}$ , since  $A^4 \neq 0$ . However, when  $k = 4$  and  $n$  is sufficiently large, we conjecture the second part of Theorem 2 is still true.

When  $k = 3$ , Theorem 2 does not hold, which is shown by the following example. Let

$$T'_3 = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

and

$$A = \begin{bmatrix} T_3 & T'_3 & T_3 & \cdots & T_3 \\ T_3 & T_3 & T_3 & \cdots & T_3 \\ T_3 & T_3 & T_3 & \cdots & T_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_3 & T_3 & T_3 & \cdots & T_3 \end{bmatrix} \in M_{3t}\{0, 1\}.$$

Denote  $(b_{ij}) = A^3$ . Then

$$b_{ij} = \begin{cases} 1, & \text{if } i = 3s + 1, j = 3l \text{ for } s \in \{0, \dots, t-1\}, l \in \{1, \dots, t\}; \\ 0, & \text{otherwise.} \end{cases}$$

Therefore,  $D(A)$  is an  $\mathcal{F}_3$ -free digraph and

$$ex(3t, \mathcal{F}_3) \geq f(A) > f(\Pi_{t,3}).$$

When  $k = 2$ , by [14, Theorem 2] we can deduce

$$ex(n, \mathcal{F}_2) = \begin{cases} \frac{n^2+4n-5}{4}, & \text{if } n \text{ is odd,} \\ \frac{n^2+4n-8}{4}, & \text{if } n \text{ is even and } n \neq 4, \\ 7, & \text{if } n = 4. \end{cases}$$

The set of extremal digraphs  $Ex(n, \mathcal{F}_2)$  is not known.

We leave the problems of determining  $ex(n, \mathcal{F}_3)$  and  $Ex(n, \mathcal{F}_k)$  for  $k = 2, 3, 4$  for future work.

## Acknowledgement

The first author is grateful to Professor Yuejian Peng for helpful discussions on extremal graph theory. The research of Huang was supported by the NSFC grant 11401197 and a Fundamental Research Fund for the Central Universities.

## References

- [1] B. Bollobás, Extremal graph theory, Handbook of combinatorics, Vol. 2, 1231-1292, Elsevier, Amsterdam, 1995.

- [2] J.A. Bondy, U.S.R. Murty, Graph Theory, in: GTM, vol. 244, Springer, 2008.
- [3] W.G. Brown, P. Erdős, M. Simonovits, Extremal problems for directed graphs, J. Combinatorial Theory Ser. B 15 (1973) 77-93.
- [4] W.G. Brown, P. Erdős, M. Simonovits, Algorithmic solution of extremal digraph problems, Trans. Amer. Math. Soc. 292 (1985) 421-449.
- [5] W.G. Brown and F. Harary, Extremal digraphs, Combinatorial Theory and its Applications, Colloq. Math. Soc. Janos Bolyai 4 (1970) I, 135-198.
- [6] W. G. Brown, M. Simonovits, Extremal multigraph and digraph problems, Paul Erdős and his mathematics, II (Budapest, 1999), 157-203, Bolyai Soc. Math. Stud., 11, Jnos Bolyai Math. Soc., Budapest, 2002.
- [7] F. A. Firke, P. M. Kosek, E. D. Nash, J. Williford, Extremal graphs without 4-cycles, J. Combin. Theory Ser. B 103 (2013) 327-336.
- [8] Z. Huang, X. Zhan, Digraphs that have at most one walk of a given length with the same endpoints, Discrete Math. 311 (2011) 70-79.
- [9] H. Jacob, H. Meyniel, Extension of Turán's and Brooks' theorems and new notions of stability and coloring in digraphs, Annals of Discrete Mathematics, 17 (1983) 365-370.
- [10] V. Nikiforov, Some new results in extremal graph theory, Surveys in combinatorics 2011, 141-181, London Math. Soc. Lecture Note Ser. 392, Cambridge Univ. Press, Cambridge, 2011.
- [11] M. Tait, C. Timmons, Sidon sets and graphs without 4-cycles, J. Comb. 5 (2014) 155-165.
- [12] P. Turán, Egy grafelmeletsi zelsbertekfe ladatrbl, Mat. Fiz. Lapok 48 (1941),4 36-452.
- [13] P. Turán, On the theory of graphs, Colloq. Math. 3 (1954) 19-30.
- [14] H. Wu, On the 0-1 matrices whose squares are 0-1 matrices, Linear Algebra Appl. 432 (2010) 2909-2924.
- [15] X. Zhan, Matrix theory, Graduate Studies in Mathematics 147, American Mathematical Society, Providence, RI, 2013.